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REMOVAL OF VOLATILE ORGANICS FROM HUMIDIFIED AIR STREAMS BY ABSORPTION

R.W. COUTANT, T. ZWICK, B.C. KIM

BATTELLE COLUMBUS 505 KING AVENUE COLUMBUS OH 43201

DECEMBER 1987

FINAL REPORT

JULY 1985 - MARCH 1987



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The Air Force frequently relies on air-stripping technologies to remove organic chemicals from groundwaters contaminated from fuel and solvent spills. Although air stripping is extremely efficient at removing contaminants from the groundwater, these contaminants are only transferred into the air and in several states, air pollution controls are also required. Activated carbon beds are one potential emissions control under study. The objective of this study was to determine the effects of contaminant concentration, humidity, and chemical competition on the sorption performance of activated carbons. Based on laboratory results, a preliminary cost comparison was made for heated and unheated carbon beds. Volatile organics of interest included benzene, ethyl benzene, toluene, xylenes, trichloroethylene and 1,1-dichloroethylene.						
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PREFACE

This report was prepared by the Battelle Columbus Division, 505 King Avenue, Columbus OH 43201, under subtask 1.01 of Contract Number F08635-85-C-0122, for the Air Force Engineering and Services Center, Engineering and Services Laboratory (AFESC/RDVW), Tyndall Air Force Base FL 32403-6001.

The report summarizes work done between 1 July 1985 and 13 March 1987. The HQ AFESC/RDVW program manager was Mr Douglas C. Downey.

This report has been reviewed by the Public Affairs (PA) office and is releasable to the National Technical Information Service (NTIS). At NTIS, it will be available to the general public, including foreign nationals.

This technical report has been reviewed and is approved for publication.

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SECTION I

A. OBJECTIVE

The objective of this program was to determine the effects of VOC concentration, temperature, species competition, and humidity on the sorption performance (capacity and kinetics) of activated carbons and possibly other sorbents for the removal of selected VOCs. VOCs of interest include benzene, ethylbenzene, toluene, xylenes, trichloroethylene, and 1,1-dichloroethylene. Concentrations of interest are in the range of 30 to 300 mg/m 3 (nominally 7 to 70 ppmv).

B. BACKGROUND

Air stripping is a widely used cleanup technique for removing volatile organic contaminants (VOCs) from groundwater. The effluent air stream is usually vented directly to the atmosphere. Although the resulting VOC concentrations in the air are relatively low, there is increasing pressure from both state and federal agencies to reduce the air pollution potential of such processes. The Air Force is considering the use of such stripping processes to remove VOCs such as benzene, ethylbenzene, and trichloroethylene from groundwater.

Adsorption of a contaminant from a stream of gas passing through either a fixed or fluidized bed of sorbent is a dynamic process that depends on:

- 1. The equilibrium distribution of sorbate in the vapor and adsorbed phases.
- 2. The dynamics of vapor transport:
 - (a) to particle surfaces, and
 - (b) within the micropore structure of the sorbent particles.
- 3. The rate of flow through the bed.

The equilibrium between sorbate and the adsorbed phase is a function of the concentration of the sorbate in the gas phase; this is usually expressed in terms of an adsorption isotherm. Adsorption isotherms can have several different shape characteristics depending on the specific types of interactions (surface adsorption, multilayer adsorption, pore condensation, etc.), and these can generally be categorized in terms of Brunauer's classification system (Reference 1). For example, the adsorption of water on activated carbons usually follows Brunauer's (BET) Type II isotherm with hysteresis, illustrated in Figure 1 in the form of a plot for the amount adsorbed (arbitrary units) versus the ratio of the partial pressure to the equilibrium vapor pressure. This type of isotherm shows three distinct regions:

- 1. At low relative pressures (below the knee), adsorption occurs primarily on the free surfaces of the sorbent.
- 2. At intermediate pressures, the isotherm is relatively flat, with only multilayer adsorption occurring.
- 3. At some critical relative pressure (0.6 in Figure 1), depending on the micropore size distribution, capillary condensation begins to occur, with the result that the micropores become filled with liquid water. This process is possible because of the small size of the pores and hence the small radius of curvature of the liquid surface.

This behavior may inhibit the kinetics of adsorption of other components (especially those present at low concentrations) because of the fact that pore surfaces can become blocked by liquid water. In such cases, adsorption of the trace components may still occur if they are soluble in water, but this adds more resistance to the overall transport process.

Transport processes within the sorbent bed are determined primarily by the particle size and the pore structure of the particles. Large particles yield large intraparticle spaces, and decrease the efficiency of contact between the gas and the sorbent bed. On the other hand, very small intraparticle spaces cause high pressure drops across the bed, and some tradeoffs are necessary. Transport within a particle occurs solely by diffusion. Thus, large pores provide the best access to the internal surfaces

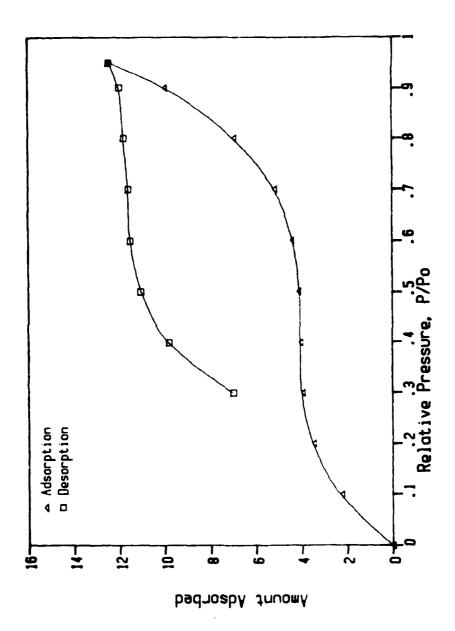


Figure 1. Typical BET Type II Isotherm.

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of the particles. On the other hand, smaller pores provide more surface area per unit porosity and therefore provide greater sorption capacity per unit weight of sorbent. With pore sizes that are smaller than about twice the mean free path of the sorbate molecules however, the effective diffusivities of the sorbate molecules become smaller than their free space diffusivities, and their access to the sorbent surface becomes kinetically limited. In the extreme examples of such cases, the sorbent may have a large equilibrium capacity for the sorbate, but will not perform well under dynamic sorption conditions, i.e., when the flow rate through the bed is faster than the speed at which the sorbent can accept the sorbate.

In practical testing and evaluation of sorbent beds, it is therefore important that both the equilibrium and kinetic parameters be evaluated so that appropriate tradeoffs can be considered for development of a system that is appropriate for a given task. The most commonly used engineering approach involves the use of the Wheeler model (or one of its several modifications) of bed permeation (Reference 2). Experimentally, the approach involves the measurement of bed breakthrough times (t_b) for several different bed weights (W), and the data are then correlated using

$$t_b = \frac{W_e}{C_i Q} \left(W - \frac{dQ}{k} \ln \frac{C_i}{C} \right)$$

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where W_e is the equilibrium bed loading (g/g) at the inlet concentration C_i (g/L), Q is the volumetric flow rate (L/min), d is the bed density (g/L), Q is the overall rate constant (min^{-1}) , and Q is the outlet gas concentration at time Q0. We/Q1 defines a point on the adsorption isotherm at Q1, and at very low concentrations, where the isotherm is approximately linear, this ratio defines the slope of the isotherm. Inasmuch as this slope is not constant over the whole isotherm (see Figure 1), it is important that bed performance be measured at concentrations expected to prevail under normal operating conditions. In the case of VOC removal from humid air streams, it is therefore necessary to determine sorption behavior at concentrations in the range of interest $(30 \text{ to } 300 \text{ mg/m}^3)$. For the VOCs of interest to

this program, this concentration range will yield relative pressures, P/P_0 of the order of 10^{-8} to 10^{-5} .

The BET isotherm, illustrated above for the adsorption of water vapor on carbon, is not well suited for description of the adsorption process for VOCs at these low levels of P/P_0 . For such cases, the Dubinin-Radushkevich isotherm, viz.

$$\frac{W_v}{W_o} = \exp - \left[B \left(\frac{T}{b} \right)^2 \left(\log^2 \frac{P}{P_o} \right) \right]$$

has proven of much greater utility (Reference 3). In this equation, W_V is the volume of condensed adsorbate, W_O is maximum volume available for sorbate condensation, B is a constant that is characteristic of the adsorbent, and b is an affinity coefficient that compares the strength of the adsorptive interaction with some reference adsorbate. Jonas et al (op. cit.) have shown that values of b for different sorbates can be correlated with their electronic polarizabilities. Therefore, once a particular adsorbent has been characterized with respect to a reference adsorbate (i.e., once B is determined for the adsorbent), then the adsorption behavior of that sorbent towards other sorbates can be predicted. More recently, Jonas and co-workers (Reference 4) have extended this approach to prediction of carbon adsorption performance for binary vapor mixtures.

C. SCOPE

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Ten commercially available carbon sorbents were evaluated for ability to adsorb selected VOCs. The more promising of these sorbents were subjected to detailed adsorption testing as a function of temperature, flow rate, sorbate composition, and relative humidity. Results were correlated using the Dubinin-Radushkevich isotherm and the Wheeler bed permeation model, and a computer-based predictive model was developed. Based on results obtained, an economic assessment was made for several possible engineering options for carbon-based cleanup of VOC contaminated groundwater. It is concluded that air stripping followed by purification of the stripper air is more economical than direct contact of the well water with activated carbon.

SECTION II EXPERIMENTAL APPROACH

A. GENERAL

The approach taken in this program can be divided into a series of subtasks:

- Adsorbent screening and selection. Ten activated carbons were considered initially as candidate sorbents. These sorbents were subjected to a series of measurements to determine their relative adsorption capacities, adsorption kinetics, and water adsorption isotherms. Based on the results of these tests and considerations of sorbent costs, the list of sorbents to be considered further was limited to the five that appeared to be most promising. This list was further reduced during subsequent tests until only one sorbent remained for the final series of experiments.
- Single-component studies. Adsorption studies were conducted using representative VOCs one at a time. These studies were conducted using various concentrations at ambient temperature and low (<5 percent) humidity to provide an optimum performance baseline set of data.
- Multiple-component studies. The adsorption behavior of various combinations of the VOCs of interest were determined at low humidities.
- Humidity effect studies. The adsorption of VOCs of interest was studied at various humidity levels. These studies were conducted with both single- and multiple-component feedstocks at ambient temperature. Finally the effect of increased temperature on adsorption of multiple-component mixtures of VOCs from humidified feedstocks was evaluated.
- Economic assessment. A preliminary process design and economic analysis was performed to obtain capital and operating costs for treatment of well water contaminated with VOCs by activated carbon adsorption. A total of nine treatment options were included in the analysis to assess vapor-phase adsorption versus liquid-phase adsorption; effects of contaminant levels in the well water; and effects of relative humidity levels in the air stream feed to the absorber.

Throughout the course of the program, data were analyzed in terms of the Dubinin-Radushkevich and Wheeler (DRW) models. To facilitate these

analyses, a computer model incorporating the DRW concepts and using ideal solution theory to estimate multiple-component effects was developed. The mathematical development of this model is described in Appendix A.

B. APPARATUS

A schematic representation of the experimental apparatus used for most of the experiments conducted on this program is shown in Figure 2. With this system, a metered flow of gas containing the VOCs is passed through the sorbent bed at controlled levels of humidity and temperature. The effluent then passes through a gas sampling valve to a continuously operating flame ionization detector (FID). With this configuration, breakthrough of the VOCs was detected by the FID detector. When using multiplecomponent sorbate mixtures, repeated samples of the effluent stream were automatically routed to a gas chromatograph for analysis. Calibrations of the FID and the gas chromatograph were performed by bypassing the sorbent bed. With this system, complete breakthrough curves could be generated, and, when necessary, desorption curves could be observed. For those experiments requiring high humidity, a Nafion dryer was installed at the bed outlet. This avoided problems associated with condensation and subsequent aqueous phase absorption of VOCs and interference of water with the analysis procedures.

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C. SORBENT BEDS

Sorbent beds were prepared in 1/4-inch stainless steel tubes containing 0.1-0.8 grams of carbon depending on the density of the carbon and the depth of bed desired. Before each use, beds were baked at 180-200 degrees Centigrade with nitrogen passing through the bed. Baking was continued until no evidence of hydrocarbon elution was seen with the FID.

In initial tests, fresh beds were prepared for each experiment. These tests included thermal desorption measurements made at the completion of each adsorption run. Subsequent tests with the thermally regenerated beds showed no detectable differences in adsorption performance. A limited

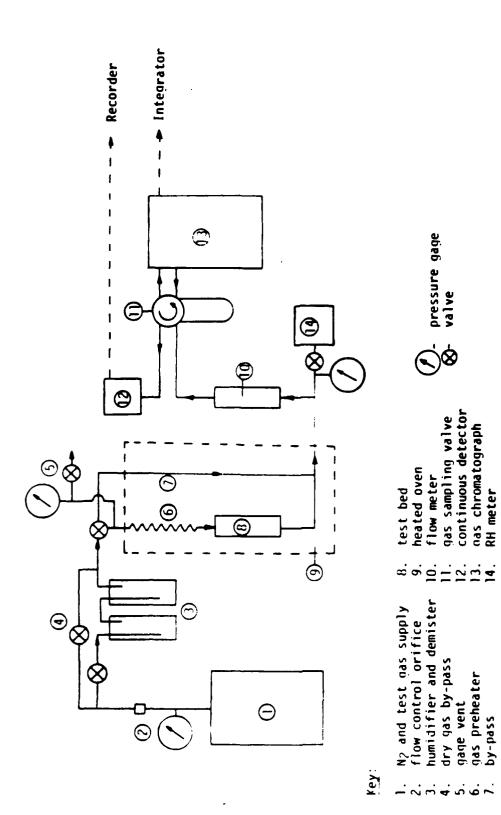


Figure 2. Schematic of Sorbent Evaluation Apparatus.

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number of regeneration trials were conducted using steam regeneration of the beds, but no particular advantage, other than the use of lower temperatures was found for this procedure. Subsequent experiments were conducted using thermally regenerated beds, with occasional comparisons being made with fresh beds. Deterioration of bed performance occurred only once, after several tens of regenerations.

D. CARBONS

Activated carbons considered initially for this program are cited in Table 1. These included both conventional carbons and recently developed specialty carbons.

TABLE 1. LIST OF SORBENTS USED IN SCREENING TESTS

Sorbent	Туре	Comments	
Activated Carbons:			
SK-4	nut shell		
LCL	coconut shell		
WV-B	coal base		
CT	coconut shell		
Specialty Carbons:			
Graphpac	graphitized carbon	area - 100 m²/g	
Carbosphere	carbon "mole sieve"	1000 m ² /g; low water retention	
Spherocarb	carbon "mole sieve"	similar to Carbosphere	
Carbopack	graphitized carbon	similar to Graphpac	
Carbosieve G	low-density carbon		
Carbosieve S-11	high-density carbon	ca.1000m ² /g	

E. ADSORPTION ISOTHERMS

Low-concentration data for the Dubinin-Radushkevich isotherms were derived directly from the bed-permeation experiments described above.

However, high-concentration (near saturation) capacities for the VOCs and water-adsorption isotherms were more conveniently determined gravimetrically. For these measurements, a Cahn Model RG recording microbalance was used with the following procedure:

- 1. A sample of the carbon was placed on the balance pan, and was outgassed at about 150 degrees Centigrade in a stream of dry nitrogen.
- 2. After cooling the sample to 25 degrees Centigrade, the gas flow to the sample area was switched to either a humidified stream of nitrogen or nitrogen containing a high concentration of the VOC of interest.
- 3. The sample was allowed to equilibrate with the gas stream, as judged by the balance output. During this time, the sorbate concentration was measured using either a relative humidity meter for water concentrations or a gas chromatograph to monitor the VOCs.
- Steps 2-3 were then repeated with successively higher sorbate concentrations.

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SECTION III RESULTS AND DISCUSSION

A. SCREENING TESTS

Each of the 10 carbons cited in Table 1 was subjected to an initial set of screening tests that consisted of determining: (a) breakthrough curves at low (<5 percent) and high (85-90 percent) humidities for both 1,1-dichloroethylene and benzene; (b) thermal desorption efficiencies; and, (c) water adsorption isotherms at ambient temperature. Detailed results of these measurements are given in Appendix B. Table 2 summarizes these measurements in terms of: (a) relative adsorption capacities; (b) relative standard deviations for the breakthrough curves; (c) water adsorption capacity at saturation; and (d) relative humidity required for 50 percent saturation of the carbon. Capacities were calculated both by total integration of the desorption curves and by using the 50 percent breakthrough time and assuming a symmetrical breakthrough curve. The former approach is considered more accurate, but the two methods agreed to within a few percent for all runs.

The data in Table 2 indicate that the two Carbosieve carbons consistently yield the highest capacities, regardless of the exposure condition. The kinetics for these two carbons, as judged from the standard deviations, also appear reasonably good, although there is more scatter apparent in these numbers than in the capacity data. CT was clearly the best of the nonspecialty carbons, while WV-B was one of the poorer performers. The capacities of Graphpac GB and Carbopack C were so low that use of these two carbons was rejected very early. Therefore, not all of the screening tests were completed with these carbons.

The water-adsorption isotherms for the eight more active carbons (see Appendix B) are generally similar, but some differences can be noted. For example, WV-B absorbs more water at 70 percent humidity than does Spherocarb at near saturation. CT, SK-4, Spherocarb, Carbosphere, and Carbosieve S-11 all have water capacities that are significantly lower than those of Carbosieve G, LCL, and WV-B.

TABLE 2. RELATIVE SORBENT PERFORMANCE

		C/C	maxa			Smi	n/s ^b			RH
	D	CE		zene		CE	<u>Ben</u>	zene	Cwater,	at 50%
Sorbent	DC	Ma	D	W	D	W	D	W	mg/g	Capacity
SK-4	0.63	0.58	0.57	0.63	0.41	0.32	0.32	0.18	306	49
Carbosieve										
S-11	1.00	1.00	0.98	1.00	1.00	0.65	0.20	0.38	346	38
Graphpac GB	0	0	0	0	NA	NA	NA	NA	NA	NA
Carbosphere	0.68	0.70	0.77	0.69	0.35	0.34	0.50	0.64	325	55
Carbopack C	0	0	0	0	NA	NA	NA	NA	NA	NA
WV-B	0.26	0.38	0.58	0.48	0.38	0.31	0.16	1.00	528	70
Spherocarb	0.63	0.85	0.76	0.70	0.48	0.30	1.00	0.12	255	6 0
LCL	0.53	0.45	0.71	0.62	0.15	1.00	0.32	0.72	410	62
СТ	0.76	0.94	0.73	0.73	0.25	0.41	0.41	0.51	323	56
Carbosieve G	0.76	0.75	1.00	0.87	0.58	0.50	0.52	0.82	476	44

 $^{^{}a}\text{C}$ = sorption capacity under test conditions; C_{max} = maximum capacity observed in this series.

Figure 3 shows a scattergram combining all of the data for the desorption efficiencies measured during the screening tests. No consistent differences in desorption efficiency were noted between individual carbons. Points circled in this figure were deleted from the numerical analysis as being more than two standard deviations from the mean. The two low rejected points were observed with carbons LCL and SK-4, and were not repeated in other runs with these sorbents. The three high rejected points occurred with benzene desorption from Spherocarb and Carbosieve S-11. In the case of the former sorbent, benzene is formed from decomposition of

 b_s = standard deviation of breakthrough curve; s_{min} = minimum standard deviation observed.

CD = low humidity runs.

dW = high humidity runs.

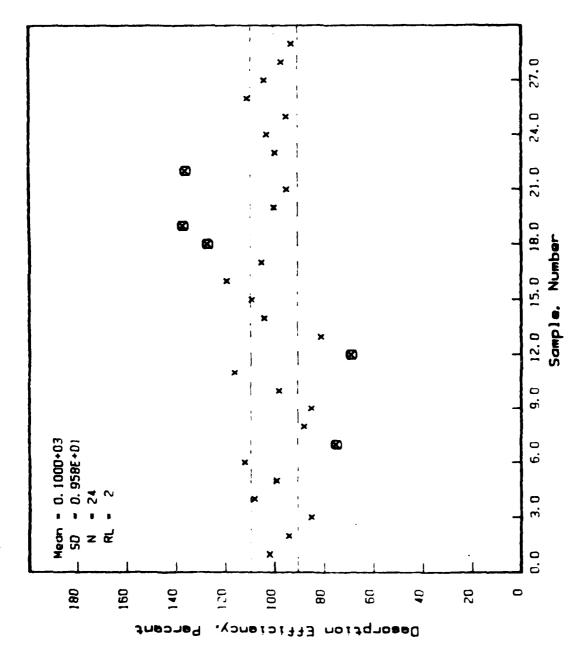


Figure 3. Thermal Desorption Efficiencies.

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incompletely pyrolyzed polymer. The high desorption efficiency with Spherocarb is, therefore, not an unexpected result.

Five of the candidate carbons were subjected to both thermal desorption and multiple steam regeneration cycles to determine if such processes would adversely affect their performance. Results of these measurements are shown in Table 3. This series of treatments had little effect on the performance of any of the carbons. Indeed, the observed changes are, for the most part, well within the expected experimental error of the measurements. Consequently, most of the remaining experiments were conducted with repeated usage of the same sorbent cartridges rather than with freshly prepared cartridges for each experiment. Spot checks on the reliability of this procedure were conducted throughout the remainder of the program, and the frequency of such repeat runs was greatest during the early stages of successive tasks.

TABLE 3. EFFECT OF THERMAL DESORPTION AND STEAM TREATMENT ON SORBENT PERFORMANCE (BENZENE AT 300 mg/m³)

Sorbent	Capacity, g/g ^a (virgin)	Capacity, g/g (treated) ^D	Percentage Change
SK-4	0.114	0.117	+2.6
Carbosieve S-11	0.195	0.180	-7.7
Spherocarb	0.149	0.151	+1.3
СТ	0.143	0.141	-1.4
Carbosieve G	0.200	0.191	<u>-4.5</u>
		Mean	-1.9 +/-4.2

^aCapacity based on 50 percent breakthrough time and input concentration level. (300 mg/m 3 x flow rate x t₅₀/bed weight.)

Based on the results of these screening tests, five carbons, CT, Carbosieve S-11, SK-4, Carbosieve G, and Spherocarb, were selected for further evaluation.

bVirgin samples exposed; thermally desorbed at 160 degrees Centigrade; steam desorbed at 100-140 degrees Centigrade; and reexposed to benzene.

B. REFERENCE DATA FOR MODEL DEVELOPMENT

The five carbons cited above were used to develop a reference data set for use with the DRW model. In these experiments, adsorption breakthrough times (defined as the time when the eluent concentration rises to 10 percent of the input concentration) and adsorption capacities were measured as a function of bed depth, feed rate, and input concentration using 1.1-dichloroethylene as the reference sorbate. As noted in the experimental section, additional capacity measurements were made at very high (P/Po - 1) 1,1-dichloroethylene concentrations using the gravimetric procedure. The combined data were then used to derive appropriate DR parameters for each of the five carbons. A detailed tabulation of the results obtained in this series of experiments is given in Appendix C. Initial estimates of the rate constants indicated considerable uncertainty in that parameter (see Appendix C). Additional measurements of bed depth effects were, therefore, incorporated into the concentration effect study in an effort to gain a better overall representation of the reference case with 1.1-dichloroethylene. The apparent rate constants were quite large compared with those cited by Jonas et al. This can be attributed to the much smaller carbon particles being used in the current study. Jonas found apparent rate constants of about 1000 min^{-1} with carbon particles having mean diameters of 0.268 cm. The current work is being conducted with 60-80 mesh (d = 0.0216 cm) particles. Because the transport process to and within the particles is diffusion-limited, the rate of transport should be inversely proportional to the particle diameter. Therefore, we would expect the rate constants for the current work to be of the order of 10,000 min⁻¹, with minor variations due to the internal structures of the different carbons. To make full use of all the data, the Wheeler equation was used along with the measured capacities for each experiment to calculate an apparent rate constant for each experiment. These values were then grouped for each sorbent, and the best value was determined for each sorbent. These results are shown in Table 4.

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TABLE 4. SUMMARY OF RATE CONSTANTS

Sorbent	Rate Constant, min-1	RSD, %
Carbosieve S-11	2.14 x 10 ⁴	21
СТ	1.86 x 10 ⁴	22
SK-4	1.23×10^4	19
Carbosieve G	1.70×10^4	18
Spherocarb	1.20×10^4	26

The apparent rate constants are of the right magnitude compared with those measured by Jonas. Although the uncertainties are large, with this large rate constant, the contribution of the kinetic term to the breakthrough time is relatively small, i.e., the breakthrough time is relatively insensitive to the exact value of the rate constant. (Conversely, the calculated rate constants are sensitive to minor variations in the breakthrough times.)

Figure 4 shows an example of the plot used to derive the DR parameters for CT. Table 5 summarizes the DR parameters derived from the data included in this part of the study. Table 6 summarizes the precision and accuracy of application of the DR isotherm to the reference data for 1,1-dichloroethylene.

TABLE 5. DUBININ-RADUSHKEVICH PARAMETERS

Sorbent	1n Wo	+/- a	k x 10 ⁸	+/- (x 10 ⁸)a
Carbosieve S-II	6.26	0.039	5.03	0.10
CT	6.05	0.056	5.02	0.16
SK-4	5.98	0.055	5.60	0.16
Carbosieve G	6.36	0.045	5.92	0.12
Spherocarb	6.08	0.049	5.39	0.14

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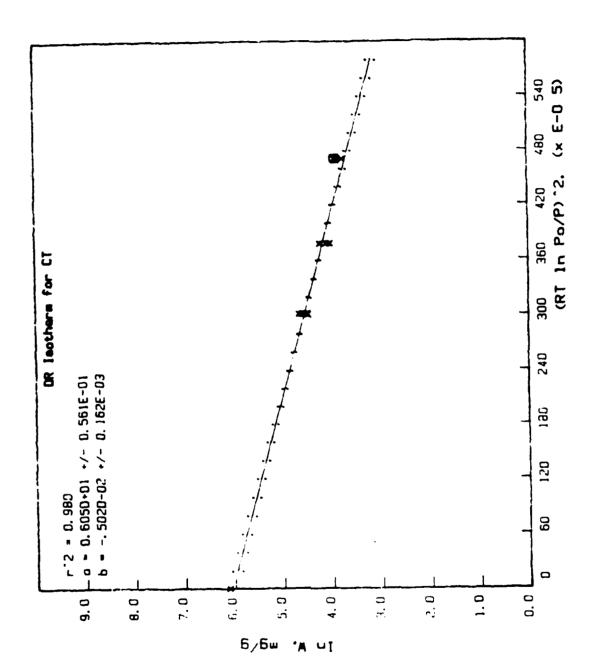


Figure 4. Dubinin-Radushkevich Plot for 1,1-Dichloroethylene on CT.

TABLE 6. SUMMARY OF PRECISION AND BIAS OF DRW REFERENCE DATA

	t	10	Capacity, mg/g	
Sorbent	pa	Вр	p	B
Carbosieve S-11	9.31	-1.49	10.0	-2.56
СТ	19.3	5.41	11.5	-2.27
SK-4	27.6	8.92	9.37	-0.16
Carbosieve G	14.9	10.1	7.80	0.54
Spherocarb	24.3	-11.4	10.2	-0.95

apprecision defined as root mean square percentage difference between predicted and measured t_{10} or capacity.

 $^{\text{b}}\textsc{Bias}$ defined as average percentage difference between predicted and measured t_{10} or capacity. (A negative bias indicates low predicted values.)

C. SINGLE COMPONENT VOC ADSORPTION

Additional bed permeation experiments were conducted using various combinations of the five candidate sorbents at various bed depths for adsorption of benzene, trichloroethylene, toluene, o-xylene, and ethylbenzene. Detailed results for these experiments are given in Appendix D. The DRW parameters derived from the reference data set with 1,1-dichloroethylene were used to estimate values of t_{10} and the adsorption capacities for each run. The calculated and measured results were then compared. Application of the DRW model to compounds other than the reference chemical is described in Appendix A. Briefly, two adjustments to the reference parameters are required:

- 1. The saturation capacity, Wo, must be adjusted to accommodate the difference in density between the reference chemical and the test chemical.
- 2. The affinity coefficient for the test chemical must be calculated relative to that of the reference chemical using the ratios of their electronic polarizabilities.

Appropriate parameters for estimation of the affinity coefficients of the test VOCs are given in Table 7. The results of application of the DRW model to the single component data are summarized in Table 8.

TABLE 7. SORBATE PROPERTIES FOR DR CORRELATION

WAYNER BOXDON SANS

Chemical	Mwa	P _o , mg/m ³ (x 10 ⁻⁵) @ 25C	₫Þ	nC	ped	P _e /P _{eDCE}
1,1-Dichloro- ethylene	96.94	31.9	1.218	1.425	20.35	1.00
Trichloro- ethylene	131.39	5.07	1.464	1.477	25.37	1.25
o-Xylene	106.17	0.353	0.880	1.506	35.81	1.76
Toluene	92.15	1.34	0.867	1.496	31.06	1.53
Ethylbenzene	106.17	0.546	0.867	1.496	35.77	1.76
Benzene	78.12	3.82	0.879	1.501	26.2 0	1.29

aMolecular weight

$$P_e = \left(\frac{n^2 - 1}{n^2 + 2}\right) \left(\frac{Mw}{d}\right)$$

Comparing the data of Table 6 with those in Table 8 shows that the indicated precision are probably inherent in the experimental technique. This could be due to variations in bed packing densities. In later experiments where the number of variables (principally the number of different carbon beds) was much more limited, the precision and apparent bias were considerably improved over the data shown in Table 8. However, even the range of bias indicated by Table 8 would probably not be unacceptable for purposes of engineering estimates of bed capacities. The biases listed in Table 8 for the t10 estimates parallel those for the capacity estimates.

bLiquid density, g/cc

CRefractive index of liquid

dElectronic polarizability

TABLE 8. APPLICABILITY OF DRW MODEL TO TEST VOCS

	······································	t ₁₀	Capacity, mg/g	
Sorbent	pa	Вр	Р	В
Benzene	12.2	7.87	9.87	6.80
Trichloroethylene	29.9	14.0	22.2	13.2
o-Xylene	31.8	-26.8	31.1	-26.6
Toluene	21.8	-17.4	18.1	-14.2
Ethylbenzene	27.5	-22.7	24.3	-19.3

aprecision defined as root mean square percentage difference between predicted and measured t_{10} or capacity.

bBias defined as average percentage difference between predicted and measured t₁₀ or capacity. (A negative bias indicates low predicted values.)

This suggests that the source of the bias is predominantly in the correlation of the affinity coefficients with electronic polarizabilities, and that a reexamination of the parameters used in this correlation might lead to improved overall prediction of capacities.

D. MULTIPLE-COMPONENT STUDIES

While considerable work has been done to characterize adsorption of individual sorbates on a wide variety of sorbents, relatively little effort has been directed towards the simultaneous adsorption of multiple sorbates. Historically, the adsorption capacities of carbons and other sorbents have been characterized in terms of one or more individual sorbates. Such data are then used as "best-case" examples for estimating bed performance.

When more than one sorbate is present in the feedstock, occurrences of both competitive and cooperative types of phenomena can make the overall description of the adsorption process quite complicated. Consider two extreme cases involving only two sorbates:

- Case 1. Two completely immiscible sorbates -- Because these sorbates are completely immiscible they cannot condense on the same volume of sorbent at the same time. They must, therefore, occupy separate zones of the sorbent bed, with the leading zone being occupied by the sorbate less strongly held. Furthermore, continued addition of the feedstock to the bed will result in expansion of the trailing zone and concomitant displacement of the leading zone. As the feed continues to the leading zone, its movement will be accelerated. This type of behavior is approximated by combinations of water and many hydrocarbons, and the phenomenon is the basis for steam desorption of carbons.
- Case 2. Two completely miscible sorbates -- If two sorbates are completely miscible and their adsorption potentials are identical (i.e., they have the same chemical functionality and vapor pressures), they will coadsorb on the same volume of sorbent without separating into zones. An example of this type of behavior is seen with the meta- and paraisomers of xylene, which are extremely difficult to separate by chromatographic means.

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With real sorbate systems, even when water is present in the feedstock, there is usually some mutual solubility of the sorbates, resulting in zone formation and at least some limited coadsorption. Even with chemically similar sorbates, such as benzene and toluene, separation into zones and accelerated movement of the leading zone are expected because of differences in vapor pressure. This implies that the greater the number of sorbates, the greater will be the differences between retention of individual sorbates in the mixture and their retention as single components. In other words, in more complex systems, less meaning is given to estimates based on single component reference systems. The only useful approach is to employ the DR isotherm to estimate adsorption capacities in each zone, using ideal solution theory to calculate the adsorbate compositions. The details of this approach are described in Appendix A.

Experiments in this portion of the program involved a single carbon. CT, and various mixtures of the six test VOCs. The target matrix of tests, based on representative conditions at selected Air Force Bases, is given in Table 9.

TABLE 9. MULTIPLE-COMPONENT TEST MATRIX

Chemical	Target Concentrations, mg/m ³ for Runs								
	1	2	3	4	5	6	7	8	
DCE	0	10	0	0	0	0	0	0	
TCE	0	50	15	0	0	0	0	0	
Benzene	15	0	40	800	50	300	300	30	
Toluene	30	0	0	100	30	300	300	300	
Et-benzene	100	0	0	0	10	300	30	30	
o-Xylene	0	0	0	0	0	300	30	30	

Results for these runs are summarized in Table 10.

These data lead to two conclusions:

- The breakthrough times are reduced considerably when more than one component is present, with the more volatile components being affected most severely.
- 2. The DRW model predictions, while not perfect, are sufficiently accurate to provide a basis for estimating behavior of other multiple-component systems (e.g., other combinations of sorbates and/or concentrations).

Because the slower moving zones in the carbon bed at least partially desorb the leading zones, the gas-phase concentrations of various

TABLE 10. MULTICOMPONENT BREAKTHROUGH TIMES

(Sorbent = 0.134 g CT)

Sorbate	C, mg/m ³	t/to ^a	t _p /t _o b	
	Run No.	1 : F = 165	cc/min	
Benzene	15	0.18	0.10	
Toluene	50	0.40	0.35	
Ethylbenzene	111	0.94	0.94	
	Run No.	2 : F = 166	cc/min	
1,1-Dichloroethylene	11	0.62	0.63	
Trichloroethylene	49	1.01	1.00	
	Run No.	3 : F = 122	cc/min	
Trichloroethylene	11	0.20	0.19	
Benzene	37	0.72	0.88	
	Run No.	4 : F = 159	cc/min	
Benzene	802	0.81	0.83	
Toluene	88	0.54	0.56	
	Run No.	5 : F = 159	cc/min	
Benzene	49	0.57	0.56	
Toluene	29	0.69	0.68	
Ethylbenzene	8	0.53	0.69	
	Run No.	6a : F = 159	9 cc/min	
Benzene	350	0.38	0.13	
Toluene	344	0.41	0.21	
Ethylbenzene	308	0.47	0.34	
o-Xylene	304	0.61	0.56	
	Run No.	6b : F = 169	5 cc/min	
Benzene	372	0.44	0.18	
Toluene	352	0.53	0.28	
Ethylbenzene	321	0.70	0.48	
o-Xylene	29	0.17	0.12	

TABLE 10. MULTICOMPONENT BREAKTHROUGH TIMES (CONCLUDED)

(Sorbent = 0.134 q CT)

Sorbate	C, mg/m ³	t/t _o a	t _p /t _o b	
Benzene	341	0.48	0.32	
Toluene	309	0.70	0.50	
Ethylbenzene	40	0.32	0.23	
o-Xylene	37	0.42	0.39	
	Run No.	8 : F = 169	cc/min	
Benzene	3 0	0.14	0.07	
Toluene	332	0.81	0.58	
Ethylbenzene	32	0.27	0.21	
o-Xylene	30	0.38	0.38	

aRatio of observed 10 percent breakthrough time to predicted single-component breakthrough time.

bPredicted ratio of multicomponent breakthrough time to single-component breakthrough time.

components in different parts of the bed are not necessarily the same as those in the feedstock. This is readily obvious from observation of the eluent concentrations in these multiple-component experiments. Figure 5 shows the eluent concentrations measured for Run 6 of this series of experiments. The concentrations of each of the three faster-moving components go through maxima that appreciably exceed their respective input concentrations. This aspect of multicomponent behavior is qualitatively predicted by the DRW model. For example, Figure 6 shows the calculated concentrations for the adsorbed phase in each bed zone for Run 6 although these are shown as smooth curves drawn through the calculated points, and are probably not very accurate, the suggested trends are significant:

1. Benzene is present to some extent in all four zones, but it forms a significant fraction of the adsorbed phase only in the last zone.

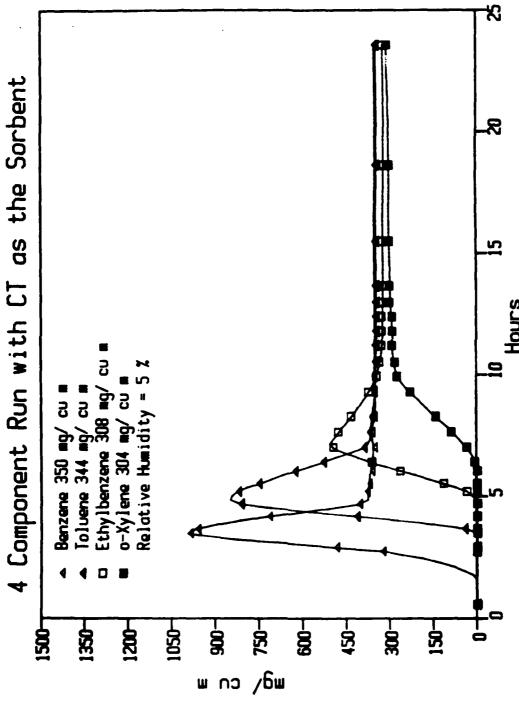


Figure 5. Eluent Concentration Profiles for Run Number 6.

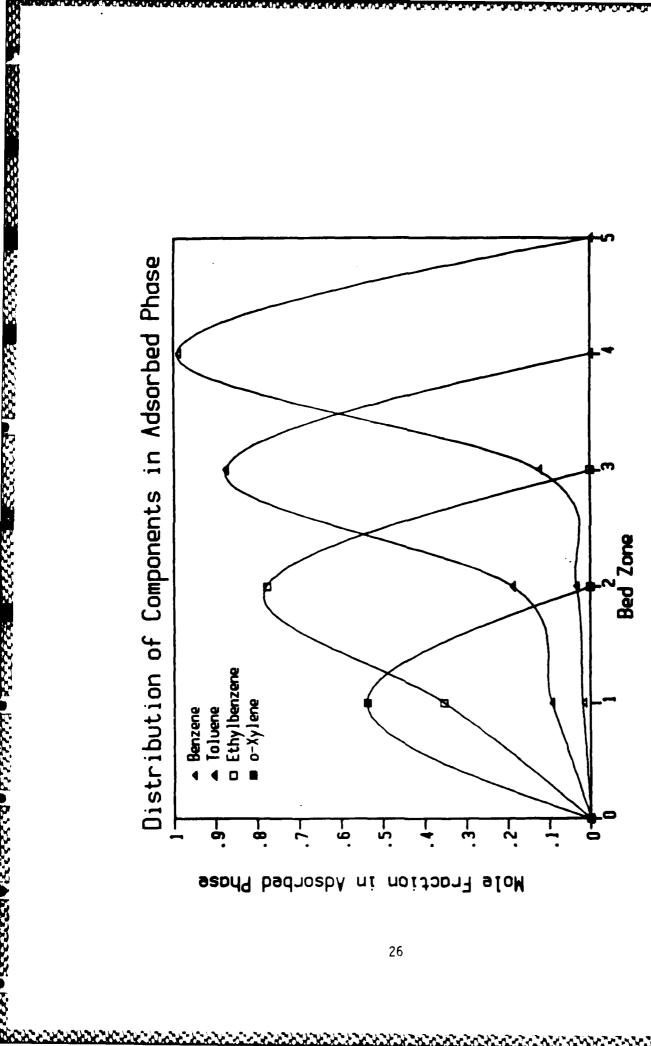


Figure 6. Calculated Adsorbed Phase Compositions for Run Number 6.

2. Toluene dominates zone 3; ethylbenzene dominates zone 2, but is also present in a significant portion of zone 1.

Thus, by the time zone 4 reaches the bed exit, it contains almost all of the benzene adsorbed during the run, and its release results in a concentration in the gas phase that greatly exceeds the input level. In this run we see examples that suggest both extremes noted above:

- Ethylbenzene and xylene coadsorb and exclude most of the more volatile components.
- 2. Benzene is largely excluded from coadsorption with the less volatile components.

Note:

These are not general conclusions, but depend on the particular combination of sorbates and concentrations.

E. RELATIVE HUMIDITY EFFECTS

Water adsorption isotherms (Figures B-1 to B-8), show that pore condensation of water on carbons generally does not occur at relative humidities below about 40-50 percent. Therefore, the use of a pseudo-Dubinin-Radushkevich isotherm to represent water adsorption offers, at best, a crude approximation. Furthermore, because most VOCs are only slightly soluble in water, the use of ideal solution theory with such solutions is inappropriate. Therefore, one cannot use the DRW model developed on this program to estimate relative humidity effects with more than semigualitative accuracy. It has been suggested (Werner) that for dual-component sorbate systems in which one of the components is water, a pseudo-DR isotherm can be used, along with the known water solubility of the second component. Such an approach is potentially useful only if sufficient information on water solubilities is available. Unfortunately, water solubilities for mixtures of VOCs are often complex functions of VOC concentrations, and complete experimental descriptions of systems of interest are not generally available. Nonetheless, it is useful to

consider the qualitative predictions of the DRW model with respect to the effect of relative humidity on VOC adsorption.

If we estimate the affinity coefficient of water using the molar refractivity correlation (see Appendix A), we find that the affinity coefficient for water is 0.24 times that of benzene or trichloroethylene and 0.15 times that of o-xylene or ethylbenzene. Any two sorbates compared will have equal adsorption potentials when the ratios of the logarithms of their relative pressures to their affinity coefficients are equal (assuming a DR isotherm). We can use this to estimate the relative pressure of VOC needed to compete on an equal basis with water vapor as function of the relative pressure of water, as shown in Figure 7.

The curves shown in Figure 7 (which are independent of the carbon) emphasize the fact that the adsorption potential of a given sorbate is a function of: (a) the equilibrium vapor pressure of the sorbate; (b) the actual vapor concentration; and (c) the affinity coefficient of the sorbate. At high values of P/P_0 , almost any VOC would be expected to be relatively unaffected by the presence of water vapor. At low P/P_0 values, sorbates having low affinity coefficients are most strongly affected by water vapor. The curves also illustrate the magnitude of the displacement effects with different VOCs at low concentrations. For example, benzene at $P/P_0 = 3 \times 10^{-6}$ (about 1 mg/m³ at 25 C) would be displaced by xylene at $P/P_0 > 2 \times 10^{-9}$ (about 6.4 x 10^{-5} mg/m³).

General conclusions concerning the effect of water vapor that can be drawn from the DRW model are:

- 1. The higher the adsorption potential for a particular component the less it will be affected by the presence of other sorbates, including water vapor.
- 2. Sorbates having relatively low affinity coefficients should show greater concentration effects in the presence of other sorbates. This means that concentration effects with o-xylene and water vapor should be less than those observed by Werner for trichloroethylene and water vapor.
- 3. There should be no differences between behaviors of different sorbates when comparison is made on the basis of equal adsorption potentials rather than on an equal concentration basis.

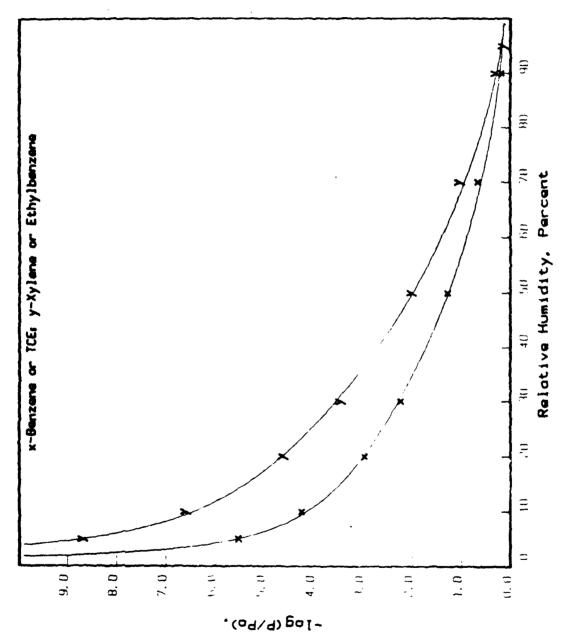


Figure 7. Concentration of VOC Required for Equal Competition with Water Vapor.

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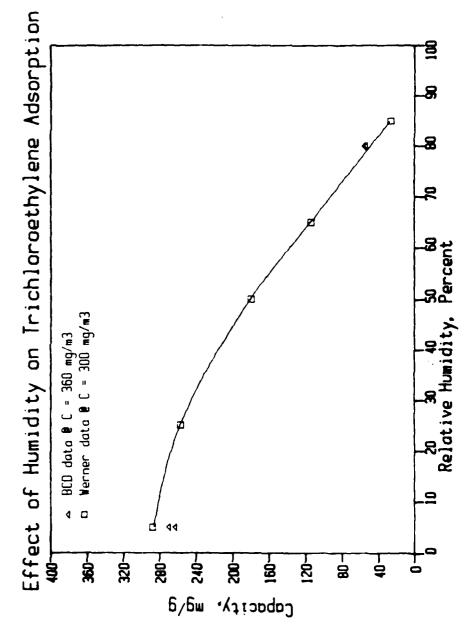
CONTRACT DESCRIPTION

Initial experiments to study the effect of water vapor on VOC adsorption on carbons consisted of replication of selected experiments performed by Werner on an earlier program for the Air Force. For these experiments, samples of the carbon used by Werner were obtained and were crushed and sieved to 60/80 mesh. A comparison of Werner's results with trichloroethylene adsorption and those obtained in the current work is given in Figure 8. This figure shows that relatively good agreement was obtained with Werner's results.

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Additional experiments were conducted at various humidities with 1,1-dichloroethylene, benzene, and o-xylene as the sorbates and CT as the sorbent. Data from these experiments are shown in Figures 9 and 10.

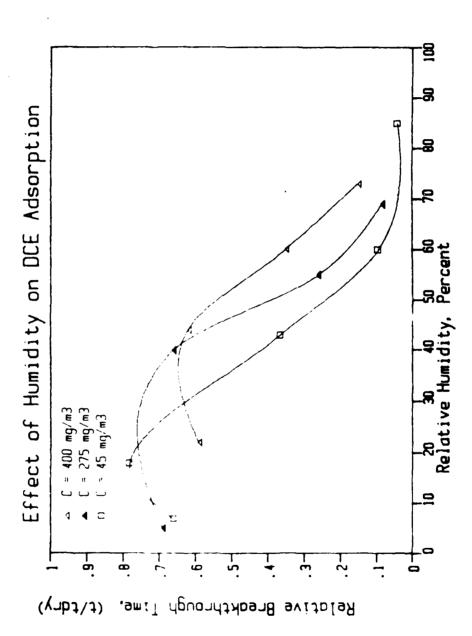
While there is somewhat more scatter in the data for benzene and 1.1-dichloroethylene than for o-xylene, it can be seen that 1,1-dichloroethylene and benzene are more severely affected by the presence of water vapor, and that significant effects on the adsorption of 1,1-dichloroethylene and benzene occur at humidities above about 30 percent. Furthermore, the lower the concentration of 1,1-dichloroethylene, the more severe the humidity effect. This agrees with Werner's findings and the general inferences based on the DRW model. Experiments were also conducted to determine the synergistic effects of temperature and humidity of the adsorption of mixtures of VOCs. In these experiments, the feedstock was humidified to approximately 75 percent RH at 25 degrees Centigrade, while the bed was operated at various temperatures from 25 to 55 degrees Centigrade. The net effect of increased temperature in the bed is to lower the effective relative humidity within the bed. Results of these runs are given in Table 11. In this table, breakthrough times are given as ratios of measured breakthrough times to those calculated for the dry system. This normalization procedure removes some of the variation in the data due to slightly different conditions used for the individual experiments. For convenience in interpretation, these data are plotted in Figure 11, which shows that xylene is affected least by the high humidity, and the two chlorinated compounds are affected most strongly. This is in agreement with the relative adsorption potentials of these compounds. All five compounds show increased retention with increased temperatures to 35-45 degrees Centigrade.



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Figure 8. Effect of Humidity on Adsorption of Trichloroethylene.

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Figure 9. Effect of Pelative Humidity on 1,1-Dichloroethylene Adsorption.

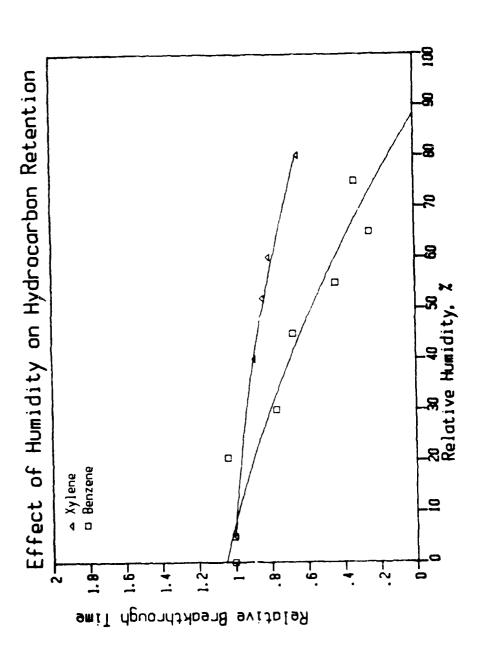


Figure 10. Effect of Relative Humidity on Adsorption of Benzene and o-Xylene.

TABLE 11. INITIAL HUMIDITY/TEMPERATURE RUNS (CARBON BED = CT)

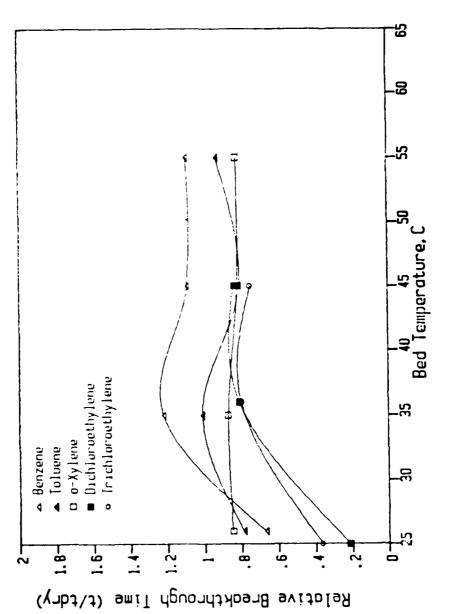
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Sorbate	C, mg/m ³	t ₁₀ t ₁₀ (cal)
Benzene Toluene o-Xylene	Run 1111; F=150 cc/mi 356 328 337	in; T = 26 C; RH = 74 ^a 0.67 0.79 0.85
Benzene Toluene o-Xylene	Run 1112; F=152 cc/mi 346 328 336	in; T = 35 C; RH = 75 1.22 1.01 0.87
Benzene Toluene o-Xylene	Run 1113; F=146 cc/mi 350 332 345	in; T = 35 C; RH = 69 1.22 0.99 0.89
Benzene Toluene o-Xylene	Run 1114; F=143 cc/mi 343 326 340	in; T = 45 C; RH = 73 1.09 0.81 0.82
Benzene Toluene o-Xylene	Run 1125; F=146 cc/mi 223 205 156	in; T = 55 C; RH = 75 109 0.93 0.82
1,1-Dichloroethylene Trichloroethylene	Run 1118; F=148 cc/mi 304 280	in; T = 25 C; RH = 70 0.17 0.35
1,1-Dichloroethylene Trichloroethylene	Run 1119; F=150 cc/mi 258 258	in; T = 25 C; RH = 65 0.21 0.36
1,1-Dichloroethylene Trichloroethylene	Run 1120; F=150 cc/mi 259 262	in; T = 36 C; RH = 69 0.78
1,1-Dichloroethylene Trichloroethylene	Run 1121; F=143 cc/mi 283 279	in; T = 45 C; RH = 66 0.84 0.75

TABLE 11. INITIAL HUMIDITY/TEMPERATURE RUNS (CARBON BED = CT) (CONCLUDED)

Sorbate	C, mg/m ³	t10t10(cal)
1,1-Dichloroethylene	Run 1122; F=148 cc/mi 293	n; T = 25 C; RH = 5
Trichloroethylene	307	0.96
	Run 1124; F=150 cc/mi	· •
1,1-Dichloroethylene Trichloroethylene	317 277	0.81 0.80

aRelative humidities measured at 25 degrees Centigrade.



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Figure 11. Effect of Increased Bed Temperature on Retention of VOCs from Humidified Gas Streams.

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SECTION IV ECONOMIC ASSESSMENT

The objective of this subtask was to provide a preliminary economic assessment of various carbon adsorption systems for treatment of well water contaminated with volatile organic compounds (VOCs). The following treatment options were included in the analysis:

- Option 1A: Air stripping of well water, followed by air cleaning with activated carbon for Case 1 contaminants listed in Table 12.
- Option 1B: Air stripping of well water, followed by air cleaning with activated carbon for Case 2 contaminants listed in Table 12.
- Option 1C: Air stripping of well water followed by air cleaning with activated carbon for Case 3 contaminants listed in Table 12.
- Option 2A: Air stripping of well water, followed by preheating of the contaminated air and cleaning of the heated air with activated carbon for Case 1 contaminants.

- Option 2B: Air stripping of well water, followed by preheating of the contaminated air and cleaning of the heated air with activated carbon for Case 2 contaminants.
- Option 2C: Air stripping of well water followed by preheating of the contaminated air and subsequent cleaning of the heated air with activated carbon for Case 3 contaminants.
- Option 3A: Direct contact of well water with activated carbon for Case 1 contaminants.
- Option 3B: Direct contact of well water with activated carbon for Case 2 contaminants.
- Option 3C: Direct contact of well water with activated carbon for Case 3 contaminants.

TABLE 12. VOC CONCENTRATION IN WELL WATER

VOC	VOC C	oncentratio	n, ppb
	Case 1	Case 2	Case 3
Benzene	100	0	1000
Toluene	100	0	1000
Ethylbenzene	100	0	1000
Xylene	100	0	1000
Trichloroethylene	0	100	0
1,1-Dichloroethylene	0	100	0

A. PRELIMINARY PROCESS DESIGN

A preliminary process design was performed to size major process equipment items for estimation of capital costs. Operating costs were estimated from utility costs, carbon usage, and capital-related costs, such as amortization and maintenance costs. A process design was based on the criteria listed below:

a. Well water:

Treatment rate: 50 gpm 12 hours/day, 365 days/year

Treatment period: 10 years

Temperature: 13 degrees Centigrade (55 degrees Fahrenheit)

b. Stripping air:

Flow rate: 335 cfm (air-to-water ratio of 50)

Temperature: 20 degrees Centigrade (68 degrees Fahrenheit)

Design procedures and results are described below.

B. AIR-STRIPPING TOWER

Packed towers are the most effective and widely used equipment for the aeration process. A packed tower with a 2-foot diameter and 22.5-foot packing height was sized on discussions with an equipment supplier (Reference 6). The superficial gas velocity in this tower is estimated at around 1.8 ft/sec, and the liquid (water) rate at around 8000 lb/hr-ft 2 . The pressure drop through 1-inch Raschig ring packing is estimated at around 0.5 inch H₂0 per foot of packing, normally found at the flooding point and, therefore, is acceptable.

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C. CARBON ADSORPTION TOWER

An adsorption tower for air cleaning was sized at 4-foot diameter by 4-foot bed depth, which holds approximately 1500 pounds of activated carbon, based on discussions with a supplier of activated carbon adsorption systems (Reference 7). The superficial gas velocity for this unit, based on an airflow rate of 335 cfm, is estimated at 27 ft/min, which is within the range of 20 to 100 ft/min of superficial gas velocity utilized normally in vapor phase system designs (Reference 7). The bed depth of 4 feet is conservative when compared with normal bed depths in the 2- to 3-foot range (Reference 7).

For a liquid-phase contact system to be utilized for direct purification of the contaminated well water without air stripping, a disposable adsorption system utilizing four disposable drum adsorbers also was selected (Reference 7). The drums are connected in two parallel lines with two drums in series in each line. Each drum contains 1000 pounds of activated carbon. The drum is approximately 44 inches in diameter and 67 inches in height. The drum is supplied with inlet and outlet pipe connections and can be easily installed and removed from the process. After the carbon in the drum is used up, the drum is taken off the process and sent to a hazardous landfill for disposal.

D. AIR HEATER

Assuming that the air stream at the outlet of the air stripper reaches the inlet water temperature of 55 degrees Fahrenheit (13 degrees Centigrade) and a 90 percent relative humidity, the partial pressure of water vapor in the air stream will be 10.0 mm Hg. Published data by Werner (Reference 8) indicate that sorption capacity of activated carbon levels off at around 25 percent relative humidity. To reduce the relative humidity from 90 percent to 25 percent, the air stream needs to be heated from 55 degrees Fahrenheit (13 degrees Centigrade) to 93 degrees Fahrenheit (34 degrees Centigrade). The theoretical energy requirement for heating the air stream is estimated at around 15,000 Btu/hr, or 4.1 kW electric.

E. ADSORPTION CAPACITY OF ACTIVATED CARBON

Based on a complete removal of VOCs by air stripping, the VOC concentration in the stripping air is estimated at 1.65 ppm by weight (2.2 mg/m³) for each of the Case 1 contaminants (i.e., benzene, toluene, ethylbenzene, and o-xylene), and for each of the Case 2 contaminants (i.e., trichloroethylene and dichloroethylene). (Note: This concentration is approximately one order of magnitude lower than was specified for the experimental phase of this work.) For Case 3 contaminants, the VOC concentration in the stripping air is estimated at 16.5 ppm by weight for each VOC. Gas-phase adsorption capacities calculated from the adsorption test results obtained in this project are given in Table 13 for the Case 1, Case 2, and Case 3 contaminants with and without heating of the stripper air (i.e., at 55 degrees Fahrenheit and 90 percent RH without heating and at 93 degrees Fahrenheit and 25 percent RH with heating). Daily carbon usage was calculated from a daily generation rate of 0.03 lb/day (for Case 1 and Case 2 contaminants) and 0.3 1b/day (for Case 3 contaminants) for each VOC and the adsorption capacity for individual VOC. The total carbon usage for a mixture of VOCs was obtained as the sum of the individual carbon requirements. The useful life of the 1500-pound carbon bed for vapor phase system was calculated from the total daily carbon usage. Calculated results are shown in Table 14. Estimated bed lives are short (i.e., less than 10 days)

TABLE 13. CALCULATED GAS-PHASE CARBON ADSORPTION CAPACITIES 1,1-Dichloroethylene ppm by wt. Temp., percent mg VOC/g carbon

VOC	VOC Conc., ppm by wt.	Air Temp., F	RH, percent	Adsorption Capacity, mg VOC/g carbor
Benzene	1.65	55	90	0.1
Toluene	1.65	55	9 0	0.5
Ethy1benzene	1.65	55	9 0	2.0
o-Xy1ene	1.65	55	9 0	3.0
Benzene	1.65	93	25	0.2
Toluene	1.65	93	25	1.2
Ethy1benzene	1.65	93	25	5.7
o-Xylene	1.65	93	25	8.7
Benzene	16.5	55	9 0	0.9
Toluene	16.5	55	9 0	4.4
Ethylbenzene	1 6. 5	55	9 0	14.6
o-Xylene	16.5	55	90	18.1
Benzene	16.5	93	25	48.9
Toluene	16.5	93	25	113.3
Ethy1benzene Ethy1benzene	16.5	93	25	152.9
o-Xylene	16.5	93	25	112.0
1,1-Dichloroethylene	1.65	55	9 0	20.0
Trichloroethylene	1.65	55	90	0.1
1,1-Dichloroethylene	1.65	93	25	40a
Trichloroethylene	1.65	93	25	0.2

aExtrapolated from trichloroethylene data.

except for Case 3 contaminants with heating of stripper air with an estimated bed life of 112 days. A regenerable system is the more economical choice when the carbon-bed life is expected to be less than 3 months (Reference 7). For the purpose of the present economic analysis, it was assumed that the carbon bed for vapor-phase adsorption is regenerated in all cases. During regeneration, steam is passed through the carbon bed to desorb the VOCs and collected outside the bed by condensation. The steam requirement is around 1.5 lb/lb carbon (i.e., around 2250 pounds of

TABLE 14. ESTIMATED CARBON-BED LIFE FOR GAS-PHASE ADSORBER

	Usage,		Life	ed Bed ^a , day
VOC	Without Heating	With Heating	Without Heating	With Heating
Case 1 Contaminants				
Benzene	300	150.0		
Toluene Ethylbenzene	60 15	25.0 5.3		
o-Xylene	10	3.4		
TOTAL	385	184	3.9	8.2
Case 2 Contaminants 1,1-Dichloroethylene Trichloroethylene	1.5 300	0.75 150		
TOTAL	302	151	5.0	9.9
Case 3 Contaminants				
Benzene	333	6.13		
Toluene	68 31	2.65		
Ethylbenzene o-Xylene	21 17	1.96 2.67	٠.	
TOTAL	439	13.4	3.4	112

aBased on 1500-pound carbon bed.

steam will be used to regenerate the 1500-pound carbon bed). The steam condensate will be contaminated with the VOCs and must be disposed of safely. The condensate can be disposed of by either: (1) the liquid can be hauled away directly, or (2) the liquid can be further treated by carbon adsorption to reduce the waste volume, and the resulting spent carbon can be hauled away.

Liquid-phase adsorption capacities were obtained from a manufacturer of activated carbons. Adsorption capacity data are given in Table 15 for Case 1 and Case 2 contaminants at 0.1 mg/L (100 ppb) for direct treatment of contaminated well waters and at 10 mg/L (10 ppm) for treatment of steam condensate resulting from regeneration of the vapor-phase adsorption

TABLE 15. LIQUID-PHASE CARBON ADSORPTION CAPACITIES AT 25 DEGREES CENTIGRADE (Reference 9)

VOC	Liquid-Phase Concentration, mg/L	Adsorption Capacity, mg VOC/g carbon
Benzene	0.1 1.0 10.0 100.0	1.4 3.4 7.2 10.5
Toluene	0.1 1.0 10.0 100.0	9.0 25.0 72.0 200.0
Ethylbenzene	0.1 1.0 10.0 100.0	9.0 53.0 310.0 800.0
o-Xylene	0.1 1.0 10.0 100.0	56.0ª 83.0ª 120.0ª 200.0ª
1,1-Dichloroethylene	0.1 10.0	1.4 17.0
Trichloroethylene	0.1	6.8 120.0

aData for p-xylene.

system, and Case 3 contaminants at 1 mg/L (1000 ppb) for direct treatment of contaminated well waters and at 100 mg/L (100 ppm) for treatment of steam condensate resulting %rom regeneration of the vapor-phase adsorption system.

Daily carbon usage was calculated from a daily generation rate of 0.03 lb/day for each VOC of Case 1 and Case 2 contaminants and a daily generation rate of 0.3 lb/day for each VOC of Case 3 contaminants, and the individual adsorption capacity. The total carbon usage for a VOC mixture

was obtained as the sum of the carbon usages for the individual VOCs. The useful life of the disposable drum adsorber, containing 1000 pounds of carbon, was calculated from the total daily carbon usage. Results shown in Table 16 indicate that a 1000-pound carbon bed would last from 9 to 498 days, depending on the VOC types, and the VOC concentrations in the liquid phase (i.e., well water or steam condensate).

TABLE 16. ESTIMATED CARBON-BED LIFE FOR LIQUID-PHASE ADSORBER

	Usage,	Carbon 1b/day	<u>L</u> ife	ed Bed ^b
VOC	0.1 mg/La	10 mg/La	0.1 mg/La	10 mg/La
Case 1 Contaminants Benzene Toluene Ethylbenzene o-Xylene TOTAL	21.4 3.3 3.3 0.5 28.5	4.17 0.42 0.10 0.25 4.94	38.8	202
Case 2 Contaminants 1,1-Dichloroethylene Trichloroethylene TOTAL	21.4 4.4 25.8	1.76 0.25 2.01	38.8	498
Case 3 Contaminants Benzene Toluene Ethylbenzene o-Xylene TOTAL	88.2 12.0 5.7 <u>3.6</u> 109.5	3.0 1.5 0.4 1.5 33.4	9.1	29.9

avoc concentration in the liquid phase.

The processes selected and described above for the various treatment options can be summarized as follows:

Options 1A, 1B, and 1C: The well water is decontaminated using a packed-bed, air-stripping tower. The off-gas from the stripping tower

bBased on 1000-pound carbon bed.

containing VOCs, is purified using a regenerable granular carbon adsorber. After the carbon in the adsorber is saturated, it is regenerated with steam. The regeneration requires approximately 1 hour, and can be scheduled during the 12-hour period when the air stripper is down. The steam condensate collected from carbon regeneration is treated with a disposable drum carbon adsorber. The condensate treatment system consists of two disposable units in series. After usage, the disposable drum containing saturated carbon is replaced with a fresh unit, and the used unit is hauled away for offsite disposal at a chemical waste landfill.

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Options 2A, 2B, and 2C: The process steps for Options 2A, 2B, and 2C are the same as for Options 1A, 1B, and 1C, except for an additional step in which the off-gas stream from the air stripper is preheated before it enters the carbon adsorber.

Options 3A, 3B, and 3C: The well water is decontaminated by direct contact with granular activated carbon. The liquid-phase adsorption system consists of four disposable drum carbon adsorber units, connected in two parallel lines with two units in series in each line. After usage, the disposable drum containing saturated carbon is replaced with a fresh unit, and the used unit is hauled away for disposal at a chemical waste landfill.

F. PROCESS ECONOMICS

Capital and operating costs were derived from various sources, including budgetary estimates provided by a manufacturer of activated carbon, equipment vendors, and published data. Operating costs were estimated with an assumption that the facility will be operated unattended, except for one operator onsite during regeneration of carbon adsorption

system and during replacement of disposable carbon adsorbers. The operating costs included the following items:

- 1. Amortized capital cost at 10 percent of capital cost per year.
- Maintenance cost, including materials and labor, at 7 percent of capital cost per year.
- 3. Utilities (electricity, steam).

- Cost of activated carbon replacement for non-regenerable adsorption systems.
- 5. Operator during adsorber regeneration and replacement.

Estimated capital and operating costs are summarized in Tables 17 and 18, respectively. Capital costs are identical for Case 1, Case 2, and Case 3 VOCs. Capital costs for the liquid-phase adsorption system without air stripping (i.e., Options 3A, 3B, and 3C) are about one-fourth of the capital costs for the vapor-phase adsorption systems that include air stripping. The lower capital costs are due to a relatively simple design based on the use of disposable carbon adsorber units.

Operating costs for the liquid-phase adsorption system are about 20 to 130 percent higher than the costs for the vapor-phase adsorption system. Therefore, we would recommend the vapor-phase adsorption system (i.e., air stripping followed by purification of the stripper air by carbon adsorption) as the more economical choice. Comparison of operating costs for Options 1A and 1B without heating of the stripper air and for Options 2A and 2B with stripper air heating shows about 10 percent reduction in cost by heating the stripper air for Case 1 and Case 2 contaminants. However, there is considerable uncertainty in this estimate because of uncertainties in the adsorption capacities at the low concentration levels that were considered in the economic analysis. Therefore, we cannot conclusively state that this estimated economic benefit of stripper air heating is significant for either Case 1 or Case 2 contaminants. Comparison of operating costs for Option 1C without heating of the stripper air and for Option 2C with stripper air heating shows about 23 percent reduction in cost by heating the stripper air for Case 3 contaminants. Heating of the stripper air is, therefore, recommended for Case 3 contaminants.

TABLE 17. ESTIMATED CAPITAL COSTS

		eatment Option	
	1A, 1B, 1C	2A, 2B, 2C	3A, 3B, 3 C
Equipment Cost, \$			
Air-stripping Tower (Reference 6)	12,500	12,500	~-
Water Pump (Reference 10)	500	500	500
Air Heater (Reference 11)		1,000	
Carbon Adsorber (air) (Reference 7)	36,000	36,000	~-
Carbon Adsorber (condensate) (Reference 9)	6,400	6,400	
Carbon Adsorber (well water) (Reference 9)			12,800
Total Purchased Equipment Cost, \$	55,400	56,400	13,300
Capital Costb, \$	105,000	107,000	25,000

aTreatment Options:

- 2A = Air stripping of water followed by preheating of air feed to carbon bed (Case 1).
- 2B = Air stripping of water followed by preheating of air feed to carbon bed (Case 2).
- 2C = Air stripping of water followed by preheating of air feed to carbon bed (Case 3).
- 3A = Direct contact of water with carbon (Case 1).
- 3B = Direct contact of water with carbon (Case 2).
- 3C = Direct contact of water with carbon (Case 3).

bCapital cost was obtained by applying a multiplication factor of 1.89 to the total purchased equipment cost (Reference 12).

	IA	18	IABLE 18.	Treatment Options 2A 28 20	ment Options	ons 2C	3A	38	30
Capital Cost, \$ Operating Cost, \$/year	105,000	105,000	105,000	107,000	107,000	107,000	25,000	25,000	25,000
Amortized Capital Cost at 10%	10,500	10,500	10,500	10,700	10,700	10,700	2,500	2,500	2,500
Mainte- nance at 7%	7,400	7,400	7,400	7,500	7,500	7,500	1,800	1,800	1,800
Electric- ity at \$0.08/kWh	1,100	1,100	1,100	2,700	2,700	2,700	009	009	009
Steam at \$10/1000 1b	2,100	1,600	2,800	1,000	800	100	!	}	!

TABLE 18. ESTIMATED OPERATING COSTS (CONCLUDED)

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				Treatm	Treatment Options	St			İ
	IA	18	10	2A	2B	30	3A	38	30
Dispos- able carbon adsorb- ers ^a	7,400	3,700	44,400	7,400	3,700	3,700 44,400 37,000 37,000 148,000	37,000	37,000	148,000
Operator at \$30/ hourb	11,200	8,800	15,400	2,600	4,500	1,100	900	900	2,400
Total Annual Cost, \$/year	39,700	33,100	81,600	34,900	29,900	66,500	42,500	42,500	155,300

**Includes disposal costs of used adsorbers containing saturated carbon.

bone operator on duty for 4 hours during each adsorber regeneration period, and for 2 hours for replacement of each disposable carbon adsorber.

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The main uncertainty in the cost estimates is associated with extrapolation of vapor-phase adsorption data that have been experimentally determined at relatively high VOC concentrations to extremely low concentrations for the purpose of process design and economic analysis. Additional vapor-phase adsorption data are needed at VOC concentrations below 10 ppm for multicomponent systems that would be directly applicable to process design. The data would be needed to refine process economics and enable the selection of an optimum treatment process for each application.

SECTION V CONCLUSIONS AND RECOMMENDATIONS

Of the various carbon sorbents considered on this program, the specialty carbons showed no special advantages over the more standard activated carbons, and would prove much less desirable than the standard carbons because of cost factors involved. Within the group of standard carbons, the CT and SK-4 were superior to LCL and WV-B with respect to their adsorption capacities. CT and SK-4 are both coconut-derived carbons produced by the same manufacturer. Differences between these two carbons may be because they are produced from different parts of the coconut.

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The model based on the Dubinin-Radushkevich isotherm and the Wheeler bed permeation equation has proven valuable for correlating adsorption of VOCs, and is especially useful for prediction of multiple component adsorption behavior. Even though the DR isotherm is not strictly applicable to the adsorption of water vapor, the model is an aid to understanding the qualitative aspects of the effects of water vapor on VOC adsorption. It is recommended that: (1) the model, in its current form, be utilized for estimation of bed requirements for adsorption of complex VOC mixtures, and (2) that consideration be given to refinement of the model with respect to relative humidity effects. Such refinement will require incorporation of a data base of solubilities for both VOCs in water and water in VOC mixtures, and improved simulation of water isotherms.

Results of the current work indicate that significant improvement in retention of VOCs, especially for the more volatile VOCs, can be obtained by reducing the effective relative humidity to below 40-50 percent. One means for accomplishing this is by increasing the bed temperature. Such increased temperature has the effect of decreasing the "dry capacities" of the VOCs by virtue of the fact that the P_0 values are increased. However, the temperature coefficient for the P_0 of water is greater than those of the VOCs examined on this program. Thus, increases in bed temperature reduce the water capacity faster than they reduce the VOC capacities. The net result is, therefore, a gain in VOC capacity relative to the "wet" system.

A preliminary process design and economic analysis based on the data obtained from the experimental program indicates that air stripping of the contaminated well water followed by purification of the stripper air by carbon adsorption is more economical than direct contact of the well water with a carbon adsorber. An economic benefit of heating the stripper air is suggested for Case 3 contaminants but less certain for either Case 1 or Case 3 contaminants. A more refined cost analysis based on additional vapor-phase adsorption data would be needed to further optimize the treatment options.

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APPENDIX A

DRW MODEL

for

MULTICOMPONENT ADSORPTION OF VOLATILE ORGANIC HYDROCARBONS ON CARBON SORBENTS

DRW MODEL

for

MULTICOMPONENT ADSORPTION OF VOLATILE ORGANIC HYDROCARBONS ON CARBON SORBENTS

A. WORKING MODEL FOR MULTICOMPONENT BED PERMEATION

Considerable work has been done in recent years to develop methods for correlation and prediction of adsorption and permeation of volatile organic hydrocarbons (VOC) in activated carbon beds. An excellent review of this work has been prepared by Werner (M. D. Werner, "Predicting Gaseous Phase Adsorption by Microporous Adsorbents," <u>CRC Critical Reviews in Environmental Control</u>, 16, 327-356, 1986). Most of these efforts have focused on the permeation behavior of single VOCs, a condition that is rarely representative of practical sorbent applications.

With the more practical case of multiple sorbates, there is competition between sorbates in the adsorption process with the result that the overall process becomes much more complex to treat in a mathematically rigorous fashion. Nonetheless, some guidelines are needed for relating the easily accessible single component data to multiple component behavior. The following is, therefore, offered as working approximation to multicomponent bed permeation.

B. PHYSICAL REPRESENTATION AND GLOSSARY OF TERMS

For purposes of this discussion, Figure A-1 represents a sorbent bed with two components, a and b, being fed to the bed at flow rate Q and concentrations C_{ao} and C_{bo} . Table A-1 identifies all abbreviations and symbols to be used in this discussion.

Component b is assumed to be more strongly adsorbed than Component a so that two zones of differing composition develop within the bed. In zone 1, both components are present at gas phase concentrations C_{i1} , and

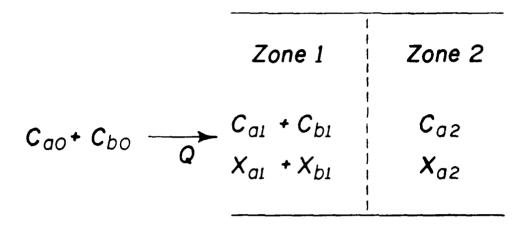


Figure A-1. Simplified Multicomponent Sorption System.

mole fractions X_{11} in the adsorbed phase. Only Component a is present in zone 2. The equilibrium between the gas phase and the adsorbed phase for each component is given by the DR isotherm, viz.

$$\frac{W_{ei}}{W_{oi}} = \exp - B \left(\frac{RT}{b_i} \ln \frac{P_{oi} X_i}{P_i} \right)^2$$
 (1)

where ideal solution behavior is assumed for the adsorbed phase [see R. J. Grant and M. Manes, "Adsorption Behavior of Binary Hydrocarbon Gas Mixtures on Activated Carbon," I&EC Fund., 5, 490-498 (1966)]. The breakthrough time for zone 1 is calculated using the Wheeler equation:

$$t_{i} = \frac{W_{ei}}{C_{i}} \left[\frac{W}{Q} - \frac{d_{b}}{k} \ln \frac{P_{oi}}{P_{i}} \right]$$
 (2)

TABLE A-1. GLOSSARY OF SYMBOLS AND ABBREVIATIONS

Symbol	Meaning	Units
i Wei Woi	sorbate index jzone index Adsorption capacity Saturation capacity	g/g g/g
Ci W Vg	Gas phase concentration Bed weight Gas phase volume	g/m ³ g m3
Vs QBTRDR bi db ds tio Pi Yi	Solid phase volume Flow rate Sorbent constant Temperature Gas constant (1.987) Dubinin-Radushkevich DR affinity coefficient Wheeler rate constant Liquid density Bulk density of bed Density of sorbent Breakthrough time (10%) Liquid vapor pressure Pressure in gas phase Mole fraction in adsorbed phase Volume fraction in adsorbed phase	m ³ /min degrees Kelvin cal/mole-deg cal/mole min-1 g/m ³ g/m ³ g/m ³ min atm atm

where the component having the longest breakthrough time is used to distinguish between zones 1 and 2. To use these equations, one must first determine X_{1j} . To do this, Grant and Manes suggest that the chemical potentials for all components in a given zone must be equal. Therefore,

$$\frac{1}{b_{11}} \ln \frac{P_{01}^{\chi} 11}{P_{11}} = \frac{1}{b_{21}} \ln \frac{P_{02}^{\chi} 21}{P_{21}} = \dots$$
 (3)

and

$$\sum_{i} x_{ij} = 1 \tag{4}$$

Equations 3 and 4 can generally be solved by the Newton-Raphson method to yield the equilibrium composition of the adsorbed phase. To proceed further, it is necessary to know the values of B and Wojj. Values of B and Wo are usually determined using a reference sorbate, and the value of B is constant for a given sorbent. The value of Wo must be adjusted for different sorbates because of differing liquid densities. In the case of multiple sorbates, care must be taken to ensure that the sum of all of the volumes occupied by the individual sorbates cannot exceed the volume implied by the value of Wo for the reference sorbate. That is,

$$W_{\text{oij}} = \left(\frac{W_{\text{o}}}{d_{1}}\right) \text{ ref}^{Y_{\text{ij}} d_{\text{lij}}} \tag{5}$$

where the values of Y_{ij} are derived from the set of X_{ij} calculated above. With these values in hand, Equations 1 and 2 can be used to determine the breakthrough time for zone 1.

The computational approach for the successive zones is similar, but with one added feature. Solutions for multiple zones, and, indeed, experimental evidence, indicate that gas phase concentrations in the successive zones are not necessarily the same as the concentrations in the input stream. If, for example, Well is very small and Well is large, then the advancement of zone 1 will necessarily be accompanied by desorption of component 1. This will have the effect of causing Cl1 to be greater than Cl2. Two approaches to accommodate this effect are:

- 1. C_{12} can be calculated from a mass balance across the boundary between zones 1 and 2.
- 2. The advance of zone 1 can be viewed in terms of a physical displacement of zone 2. (This is equivalent to assuming that the isotherm is linear between C_{11} and C_{12} .)

The first approach is preferable because of the fact that any nonlinearity in the adsorption isotherm can be accommodated through an iterative computation of the bed composition. This however is cumbersome, and the solution converges only slowly. On the other hand, the second approach is direct. It is equivalent to assuming that the <u>rates</u> of movement of successive zones are additive, i.e.,

$$(t_{12})^{-1} = (t_{21})^{-1} + \frac{W_{e12}}{C_{12}} \frac{W}{Q} - \frac{d_b}{k} \ln \frac{P_{o1}}{P_{12}}$$
 (6)

The overall process can, thus, be summarized in terms of the following computational steps:

- 1. Calculate the composition of the adsorbed phase in the first zone using Equations 3 and 4.
- 2. Use Equations 1 and 2 to determine the breakthrough time of the slowest moving component.
- 3. Eliminate the slowest moving component from the calculations and repeat step 1.
- 4. Use Equations 1 and 6 to calculate the breakthrough time for the slowest moving component of zone 2.
- 5. Repeat steps 3-5 for successive zones.

Table A-2 summarizes the results of application of this simple model in comparison with experimentally determined breakthrough times observed with selected VOCs on an activated carbon. In this case, 1,1-dichloroethylene served as the reference sorbate for determining the values of B and Wo for the sorbent, and the sorbent was an activated carbon identified as "CT." In general, the calculated breakthrough times agree reasonably well with the observed times for the 2 and 3 component systems. With the 4 component systems, the calculated results are qualitatively correct, but the discrepancies between observed and calculated times are greater, especially for the more rapidly eluting components. Figure A-2 shows a typical example (Run 6a) of the eluent profiles determined by periodic gas chromatographic analysis at the bed exit. This figure clearly illustrates the separation of components into more or less well-defined zones. Furthermore, concentrations of the early eluting components peak out at levels considerably higher than the input concentrations. This clearly indicates the effect of desorption of less strongly held components.

TABLE A-2. MULTICOMPONENT BREAKTHROUGH TIMES (Sorbent = 0.134 g CT)

Sorbate	C, mg/m ³ t/to ^a tp/to ^b
	Run No. 1 : Q = 165 cc/min
Benzene	15 0.18 0.10
Toluene	50 0.40 0.35
Ethylbenzene	0.94 0.94
	Run No. 2 : Q = 166 cc/min
1,1-Dichloroethylene	11 0.62 0.63
Trichloroethylene	49 1.01 1.00
	Run No. 3 : Q = 122 cc/min
Trichloroethylene	11 0.20 0.19
Benzene	37 0.72 0.88
	Run No. 4 : Q = 159 cc/min
Benzene	802 0.81 0.83
Taluene	88 0.54 0.56
	Run No. $5 : Q = 159$ cc/min
Benzene	49 0.57 0.56
Toluene	29 0.69 0.68
Ethylbenzene	8 0.53 0.69
	Run No. 6a : Q = 159 cc/min
Benzene	350 0.38 0.13
Toluene	344 0.41 0.21
Ethylbenzene	308 0.47 0.34
o-Xylene	304 0.61 0.56
	Run No. 6b : Q = 165 cc/min
Benzene	372 0.44 0.18
Toluene	352 0.53 0.28
Ethylbenzene	321 0.70 0.48
o-Xylene	29 0.17 0.12

TABLE A-2. MULTICOMPONENT BREAKTHROUGH TIMES (CONCLUDED)
(Sorbent = 0.134 g CT)

C, mg/m ³	t/toª	tp/to ^b
Run No. 7	: Q = 169	cc/min
341	0.48	0.32
309	0.70	0.50
40	0.32	0.23
37	0.42	0.39
Run No. 8	: Q = 169	cc/min
30	0.14	0.07
332	0.81	0.58
32	0.27	0.21
30	0.38	0.38
	341 309 40 37 Run No. 8 30 332 32	309 0.70 40 0.32 37 0.42 Run No. 8 : Q = 169 30 0.14 332 0.81 32 0.27

aRatio of observed 10 percent breakthrough time to predicted single component breakthrough time.

bRatio of predicted multicomponent breakthrough time to predicted single component breakthrough time.

C. ELUENT CONCENTRATIONS

This simple model correctly predicts several qualitative aspects of multiple component bed permeation:

- 1. While there is some tendency for sharing of the adsorbent by multiple components, each component moves through the bed at different rates. This results in the separation of sorbates and the formation of zones within which one component is dominant.
- 2. The advancement of the slower zones tends to displace the zones formed from the more rapidly moving sorbates, thus, accelerating their progress through the bed.
- 3. The ultimate result of this displacement process is the consecutive elimination of the faster moving zones from the bed.

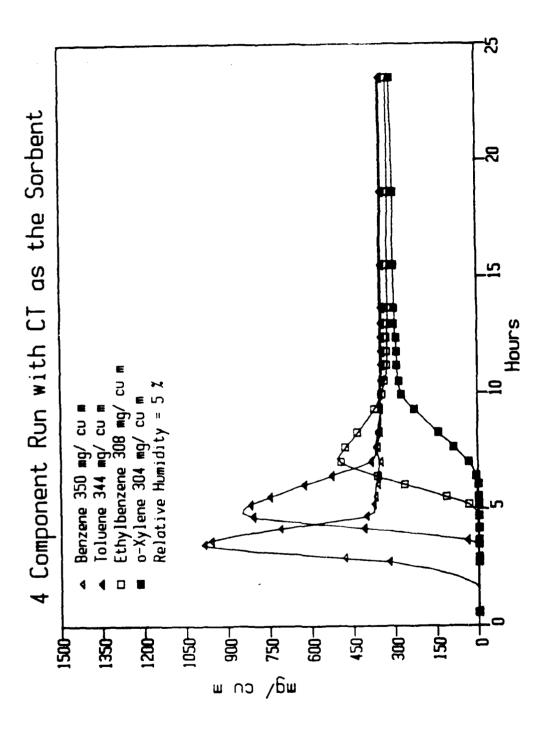


Figure A-2. Eluent Concentration Profiles for Run Number 6.

The eluent concentrations can be estimated as follows:

$$Ce_{i} = C_{ij} + \Delta C \tag{7}$$

where ΔC is obtained from a mass balance at the bed exit --

$$Q\Delta C = We_{ij}(W/t_{ij})(t_{i-1}_{i-1}-t_{ij})/t_{11})$$
(8)

where the latter factor is a correction for the fraction of the bed actually being occupied by component i at the time of its breakthrough.

D. RELATIVE HUMIDITY EFFECTS

The equations given above assume that an ideal solution is formed between the sorbates when they condense in the sorbent pores. This is a reasonable assumption for miscible sorbates, but is not a good approximation for cases where water vapor is one of the components. Two separate cases should be considered when water vapor is present:

- 1. At high relative humidities, water will tend to condense in the pore structure of the sorbent and the saturation pressure of the organic vapor is PoX_j where X_j is the liquid-liquid solubility (expressed as a mole fraction) of the organic compound in water.
- 2. At low relative humidities, the adsorbed phase is the organic and the saturation pressure of the water vapor is given by PoX_i where X_i is the liquid-liquid solubility of water in the organic.

In neither of these cases can the solubilities be estimated accurately by ideal solution theory or any other simple and straightforward process. Furthermore, although solubilities of many individual organic compounds in water are known, data on the solubilities of multiple component organic systems in water and data on the solubility of water in organic systems are quite limited. In spite of these deficiencies, the DRW model still has some utility for estimating the effects of water vapor on VOC adsorption. The approach used for this part of the code involves simulation of the water adsorption isotherm using two different DR isotherms: one set of DR

parameters is used for the low humidity side of the isotherm, and a second set of parameters is used at the high humidities. Figure A-3 illustrates how this approach approximates the water adsorption isotherm of CT. The calculated curve does not have exactly the same shape as the experimental curve. Because of the fact that the intermediate range of humidities (40-70 percent RH) are of least interest to this program, the curve fitting was done so as to best simulate the experimental data below 40 percent RH and above 80 percent RH. This approach is only semiqualitative at best, but even qualitative estimates may prove useful for the purposes of this program. An example of the utility of this approach is shown in Figure A-4. This figure reproduces the data shown in Figure 8, with an additional curve showing the calculated effect of humidity on trichloroethylene adsorption on CT (DRW parameters for Werner's carbon were not available). The calculated curve shows the same qualitative behavior indicated by the experimental data, i.e., relatively little effect of water vapor at humidities less than 30-40 percent, and a strong effect at higher humidities.

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E. COMPUTER CODE

The code used for the DRW model calculations on this program was written in MicroSoft Basic for use on IBM compatible systems. Inasmuch as the development of this code was not one of the principal objectives of the current work, the code is presented merely as a working version that has not been optimized. A listing of the code is given following this text. All necessary sorbent and sorbate parameters are included in the code, and the only input required is the specification of concentrations, temperatures, bed weight, and flow rate. Units required are specified in the prompts.

```
10 REM 'PREDICITION OF BREAKTHROUGH CURVES USING WHEELER AND DUBININ RADUSHKEVICH MODELS
20 CLS:DIM CI(10,10),X(10,10),T(10,10)
30 DEFDBL C,D,Y
40 FOR I=1 TO 7:READ A(I),BP(I):NEXT
50 FOR I=1 TO 5:READ WO(I),K(I):NEXT
60 FOR I=1 TO 5:READ D(I),KR(I):NEXT
```

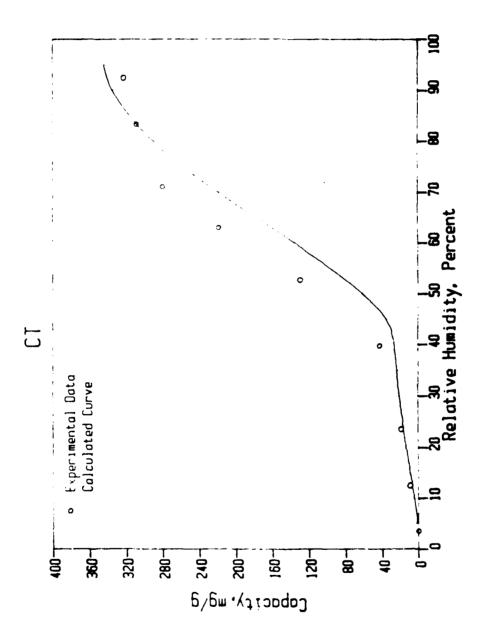


Figure A-3. Calculated Water Adsorption Isotherm.

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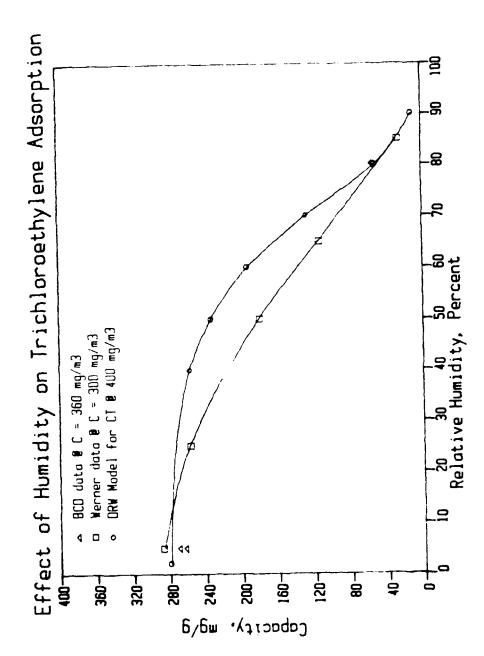


Figure A-4. Calculated Effect of Humidity on Trichloroethylene Adsorption.

```
70 FOR I=1 TO 7:READ B(I):NEXT
80 FOR I=1 TO 7:READ M(I):NEXT
90 FOR I=1 TO 7:READ DL(I):NEXT
100 FOR I=1 TO 7: READ NC$(I): NEXT
110 FOR I=1 TO 5:READ NS$(IP):NEXT
120 PRINT "Output to printer? (Y/N)"
130 A$=INKEY$: IF (A$="Y") OR (A$="y") THEN NFL=1 ELSE IF (A$="n") OR
(A$="N") THEN NFL=0 ELSE 130
140 FOR I=1 TO 5:PRINT I;NS$(I):NEXT
150 INPUT "Select one of the above sorbents by number - ".FS
160 INPUT "Number of sorbates = ",N
170 CLS:PRINT "Choose Sorbates from the following list by responding (Y/N)"
180 PRINT:FOR I=1 to 7:PRINT NC$(I)
190 A$=INKEY$:IF A$="Y" OR A$="y" THEN FL(I)=1 ELSE IF A$="n" OR
A$="N" THEN FL(I)=0 ELSE 190
200 IF FL(I)=1 THEN K=K+1
210 IF K=N THEN 220 ELSE NEXT
220 FOR I=1 TO 6: IF FL(I) THEN 230 ELSE 240
230 PRINT "Concentration (mg/m^3) of ";NC$(I);" = ";:INPUT;CI(I,1)
240 PRINT:NEXT
250 IF FL(7) THEN 260 ELSE 300
260 INPUT "Relative Humidity (%) = ":RH
270 INPUT "Input air temperature, C = ":TA:TA=TA+273
280 PO(7)=(1/760)*EXP(A(7)+BP(7)/TA):CO(7)=PO(7)*M(7)*1000000!/(.082055*TA)
290 CI(7,1)=CO(7)*(RH/100)
300 INPUT "Bed Temperature, C = ", TE:TE=TE+273:CI(7,1)=CI(7,1)*TA/TE
310 INPUT "Bed Weight, g = ",W
320 INPUT "Flow Rate, L/min = ",F
330 IF NFL THEN LPRINT N: "Component run with ":NS$(FS):" as the sorbent"
340 IF NFL THEN LPRINT "Bed weight = ";W;"g" Flow rate =
":F*1000:"cc/min":" Temperature = ":TE-273:" C"
350 IF NFL THEN LPRINT "Initial concentrations, mg/m^3"
360 FOR I=1 TO 7: IF FL(I) THEN 370 ELSE 380
370 IF NFL THEN LPRINT NC$(I);" - ";CI(I,1)
380 NEXT
390 FOR I=1 TO 7: IF FL(I) THEN 400 ELSE 470
400 PO(I)=(1/760)*EXP(A(I)+BP(I)/TE):CO(I)=PO(I)*M(I)*1000000!/(.082055*TE)
410 E(I)=1.987*TE*LOG(CO(I)/CI(I,1))
420 WO=WO(FS)+LOG(DL(I)/DL(1))
430 J=1:IF I=7 THEN GOSUB 1410
440 Q(I)=EXP(WO-K(FS)*IE-08*(E(I)/B(I))2)
450 RK(I)=KR(FS)*(M(1)/M(I))^.5:RK(I)=RK(I)*(TE/298)^1.75
460 Q(I)=1000*(Q(I)/CI(I,1))*(W/F-2.30258*D(FS)/RK(I))
470 NEXT
480 FOR I=1 TO 7:FOR J=1 TO 7:W(I,J)=W:NEXT:NEXT
490 REM 'Newton-Raphson Solution for liquid mole fraction
500 FOR J=1 TO N
510 FOR I=1 TO 7:IF FL(I)=1 then 520 ELSE 530
520 XC=I
530 NEXT
540 X(XC,J)=1:IF J>1 THEN 550 ELSE 570
550 FOR I=1 TO 7: IF FL(I) THEN CI(I,J)=CI(I,J-1)
```

```
560 NEXT
570 FOR K=1 TO 50
580 Y=1-X(XC_{*}J)
590 FOR L=1 TO XC-1: IF FL(L)=1 THEN 600 ELSE 610
600 Y=Y-(CI(L,J)/CO(L))*(CO(XC)*X(XC,J)/CI(XC,J))^(B(L)/B(XC))
610 NEXT L
620 DY = -1
630 FOR L=1 TO XC-1:IF FL(L)=1 THEN 640 ELSE 650
DY=DY-(CI(L,J)/CO(L))*(CO(XC)/CI(XC,J))*(B(L)/B(XC))*(CO(XC)*X(XC,J)/CI(XC,J))-
^(B(L)/B(XC))-1)
650 NEXT
660 DX=Y/DY:X(XC,J)=X(XC,J)-DX:IF X(XC,J)<0 THEN X(XC,J)=0
670 IF ABS(DX)<.000001 THEN 740
680 FOR L=1 TO XC
690 IF FL(L)=1 THEN 700 ELSE 710
700 X(L,J)=(CI(L,J)/CO(L))*(CO(XC)*X(XC,J)/CI(XC,J))^(B(L)/B(XC))
710 NEXT L
720 IF J>1 THEN GOSUB 1240
730 NEXT K
740 YT=0:IF NFL THEN 750 ELSE 760
750 LPRINT:LPRINT "Zone ":J
760 PRINT:PRINT "Zone ";J :IF NFL THEN 770 ELSE 790
770 FOR I=1 TO 7:IF FL(I)=1 THEN LPRINT NC$(I);" XL = ";X(I,J) ELSE
790 FOR I=1 TO 7:IF FL(I)=1 THEN PRINT NC$(I);" XL = ";X(I,J) ELSE 800
800 NEXT
810 FOR I=1 TO 7:Y(I)=X(I,J)*M(I)/DL(I)
820 YT=YT+Y(I):NEXT
830 FOR I=1 TO 7:Y(I)=Y(I)/YT:NEXT
840 FOR I=1 TO 7: IF (FL(I)=1) AND (X(I,J)>0) THEN 850 ELSE 930
850 E(I)=1.987*TE*LOG(CO(I)*X(I,J)/CI(I,J))
860 \dot{WO}=\dot{WO}(FS)+LOG(DL(\dot{I})/\dot{DL}(\dot{I})):\dot{I}F\dot{Y}(\dot{I})>0 THEN \dot{WO}=\dot{WO}+LOG(\dot{Y}(\dot{I}))
870 IF I=7 THEN GOSUB 1410
880 WE(I,J)=EXP(WO-K(FS)*1E-08*(E(I)/B(I))^2)
890 RK(I)=KR(FS)*(M(I)/M(I))^.5:RK(I)=RK(I)*(TE/298)^1.75
900 T(I,J)=1000*(WE(I,J)/CI(I,J))*(W(I,J)/F-2.30258*D(FS)/RK(I))
910 FOR JJ=1 TO J-1:T(I,J)=(1/T(I,J)+1/T(TFL(JJ),JJ))^-1:NEXT
920 F$="#####.# ":G$="#.##
930 NEXT
940 TF=0:FOR I=1 TO 7
950 IF FL(I)=1 THEN 960 ELSE 980
960 IF T(1,J)>TF THEN TF=T(1,J)
970 IF TF*T(I.J) THEN TFL(J)=1
980 NEXT
990 PFL=0:L=J-1:KF=0
1000 FOR K=1 TO L
1010 IF (T(TFL(J),J)>T(TFL(K),K)) THEN 1020 ELSE 1030
1020 KF=K
1030 NEXT
1040 IF KF THEN 1050 ELSE 1080
1050 IF NFL THEN 1060 ELSE 1070
```

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```
1060 IF NFL THEN LPRINT NC$(TFL(J));" co-elutes with zone ";KF;" C =
";CI(TFL(J),J); "WE = ";WE(TFL(J),J);" t/t0 = ";:IF NFL THEN LPRINT USING
G$;T(TFL(J),J)/Q(TFL(J)):PFL=1
1070 PRINT NC$(TFL(J));" co-elutes with zone ";KF;" C = ";CI(TFL(J),J);" WE = ";WE(TFL(J),J);" t/t0 = ";:PRINT USING
G$;T(TFL(J),J)/Q(TFL(J)):PFL=1
1080 IF NFL THEN 1090 ELSE 1100
1090 LPRINT, NC$(TFL(J)); " C = ";:LPRINT USING F$;CI(TFL(J).J)::LPRINT
"WE = ";: LPRINT USING F$;WE(TFL(J),J);: LPRINT "t = ";: LPRINT USING
F$;T(TFL(J),J);:LPRINT " t/t0 = ";:LPRINT USING G$;T(TFL(J),J)/Q(TFL(J))
1100 PRINT, NC$(TFL(J));" C = ";:PRINT USING F$;CI(TFL(J),J);:PRINT
"WE = "::PRINT USING F$;WE(TFL(J),J);:PRINT "t = ";:PRINT USING
F$;T(TFL(J),J);:PRINT " t/t0 = ";:PRINT USING G$;T(TFL(J),J)/Q(TFL(J))
1110 IF J>1 THEN GOSUB 1510
1120 FL(FTL(J))=0
1130 NEXT J
1140 IF NFL THEN LPRINT CHR$(12)
1150 END
1160 DATA 18.6,-3630,18.3,-4180,18.0,-4020,18.6,-4560,18.7,-5030,20.5
2.-5174
1170 DATA 6.26,5.03,6.05,5.02,5.98,5.60,6.36,5.92,6.08,5.39
1180 DATA 622,2.14e04,421,1.86e04,592,1.23e04,238,1.7e04,534,1.2e04
1190 DATA 1,1.25,1.29,1.53,1.76,1.76,0.267
1200 DATA 96.94,131.39,78.12,92.15,106.17,106.17,18
1210 DATA 1.218,1.464,.879,.867,.867,.880,1.00
1220 DATA "1.1-Dichloroethylene", "Trichloroethylene", "Benzene", Toluene",
"Ethylbenzene", "o-Xylene", "Water"
1230 DATA "Carbosieve S-II", "CT", "SK-4", "Carbosieve G", "Spherocarb"
1240 FOR I=1 TO 7:Y(I)=X(I,J)*M(I)/DL(I)
1250 YT=YT+Y(I):NEXT
1260 FOR I=1 TO 7:Y(I)=Y(I)/YT:NEXT
1270 FOR I=1 TO 7: IF (FL(I)=1) THEN 1280 ELSE 1390
1280 E(I)=1.987*TE*LOG(CO(I)*X(I,J)/CI(I,J))
1290 WO=WO(FS)+LOG(DL(I)/DL(1)): IF Y(I)>O THEN WO=WO+LOG(Y(I))
1300 IF I=7 THEN GOSUB 1410
1310 WE(I,J)=EXP(W0-K(FS)*1E-08*(E(I)/B(I))^2)
1320 RK(I)=KR(FS)*(M(1)/M(I))^.5:RK(I)=RK(I)*(TE/298)^1.75
1330 T(I,J)=1000*(WE(I,J)/CI(I,J))*(W(I,J)/F-2.30258*D(FS)/RK(I))
1340 T(I,J)=(1/T(I,J) +1/T(TFL(J-1),J-1))^-1
1350 DC = (2 D(FS))/(2000 - D(FS))) + (WE(I,J) - WE(I,J-1)) + (T(I,J))/((T(TFL(J-1)) + D(FS)))
1),J-1))-T(I,J)
1360 IF (DC<0) AND (ABS(DC)>CI(I,1)) THEN DC=DC/2 ELSE 1380
1370 IF DC<0 THEN 1360
1380 CI(I,J) = CI(I,J-1) + DC
1390 NEXT
1400 RETURN
1410 ON FS GOTO 1420,1430,1440,1450,1460
1420 RH=.2:WA=2.46:BA1=.601:BA2=.146:GOTO 1470
1430 RH=.365:WA=2.26:BA1=.2163:BA2=.0698:GOT0 1470
1440 RH=.3:WA=1.59:BA1=.569:BA2=.1404:GOTO 1470
1450 RH=.2:WA=2.91:BA1=.724:BA2=.1437:GOTO 1470
1460 RH=.38:WA=4!:BA1=.678:BA2=.0405:GOTO 1470
```

```
1470 IF CI(7,J)/CO(7)<RH THEN 1480 ELSE 1490
1480 WO=WO-WA:B(7)=BA1
1490 IF CI(7,J)/CO(7)>RH THEN B(7)=BA2
1500 RETURN
1510 DC = 1000*WE(TFL(J),J)*(W/F)*(T(TFL(J-1),J-1)-T(TFL(J),J))/(T(TFL(J),J)*T(TFL(1),1))
1520 C = CI(TFL(J),J) + DC :PRINT "Average eluent concentration = ";:PRINT USING F$;C
1525 IF NFL=1 THEN LPRINT "Average eluent concentration = ";:IF NFL=1
1530 RETURN
```

APPENDIX B

PRELIMINARY SCREENING DATA

AND

WATER ADSORPTION ISOTHERMS

TABLE B-1. SUMMARY OF SORBENT PERFORMANCE (1,1-Dichloroethylene at 300 mg/m³ and 5% RH)

Sorbent	Capacity, mg/g ^a	t ₁₀ , hb	sc
SK-4	78	6.85	14
Carbosieve S-11	123	12.87	5.8
Graphpac GB	0	(1 min)	NA
Carbosphere	84	`6.47′	17
Carbopack C	0	(30 sec)	NA
WV-B	32	1.98	15
Spherocarb	78	6.45	12
LCL	65	5.4	40
CT	94	5.42	24
Carbosieve G	94	3.55	10

a Capacity based on 50 percent breakthrough time and input concentration level. (300 mg/m 3 x flow rate x t50/bed weight.)

bTime to 10 percent breakthrough (note that bed weights vary).

CStandard deviation expressed as a percentage of the 50 percent breakthrough time, assuming normal distribution. $((t_{50}-t_{10})/1.28 \times t_{50}.)$

TABLE B-2. SUMMARY OF SORBENT PERFORMANCE (1,1-Dichloroethylene at 300 mg/m³ and 85% RH)

Sorbent	Capacity, mg/g ^a	t ₁₀ , h ^b	sc
SK-4	68	5.63	13
Carbosieve S-11	117	12.3	6.3
Graphpac GB	0	(2 min)	NA
Carbosphere	82	`6.77	12
Carbopack C	0	(1 min)	NA
WV-B	44	2.72	13
Spherocarb	99	7.99	14
LCL	53	4.38	4.1
CT	110	7.36	10
Carbosieve G	88	3.52	8.2

a Capacity based on 50 percent breakthrough time and input concentration level. (300 mg/m 3 x flow rate x t50/bed weight.)

bTime to 10 percent breakthrough (note that bed weights vary).

CStandard deviation expressed as a percentage of the 50 percent breakthrough time, assuming normal distribution. $((t_{50}-t_{10})/1.28 \times t_{50}.)$

TABLE B-3. SUMMARY OF SORBENT PERFORMANCE (Benzene at 300 mg/m³ and 5% RH)

Sorbent	Capacity, mg/g ^a	t_{10} , h^b	s _c
SK-4	114	11.2	5
Carbosieve S-11	195	21.6	8
Graphpac GB	0	(13 min)	NA
Carbosphere	150	15.3	3.2
Carbopack C	0	(2 min)	NA.
WV-B	114	7.18	10
Spherocarb	149	14.2	1.6
LCL	139	10.8	5
CT	143	10.1	3.9
Carbosieve G	200	8.35	3.1

^aCapacity based on 50 percent breakthrough time and input concentration level. (300 mg/m 3 x flow rate x t $_{50}$ /bed weight.)

bTime to 10 percent breakthrough (note that bed weights vary).

CStandard deviation expressed as a percentage of the 50 percent breakthrough time, assuming normal distribution. $((t_{50}-t_{10})/1.28 \times t_{50})$.

TABLE 8-4. SUMMARY OF SORBENT PERFORMANCE (Benzene at 300 mg/m³ and 85% RH)

Sorbent	Capacity, mg/g ^a	t ₁₀ , hb	s _c
SK-4	139	12.3	10
Carbosieve S-11	222	25.7	4.8
Graphpac GB	0	(10 min)	NA
Carbosphere	155	15.1	2.8
Carbopack C	0	(3 min)	NA
WV-B	107	8.1	1.8
Spherocarb	156	13.5	15
LCL	138	10.6	2.5
CT	162	11.6	3.5
Carbosieve G	193	9.08	2.2

a Capacity based on 50 percent breakthrough time and input concentration level. (300 mg/m 3 x flow rate x t_{50} /bed weight.)

bTime to 10 percent breakthrough (note that bed weights vary).

CStandard deviation expressed as a percentage of the 50 percent breakthrough time, assuming normal distribution. $((t_{50}-t_{10})/1.28 \times t_{50})$.

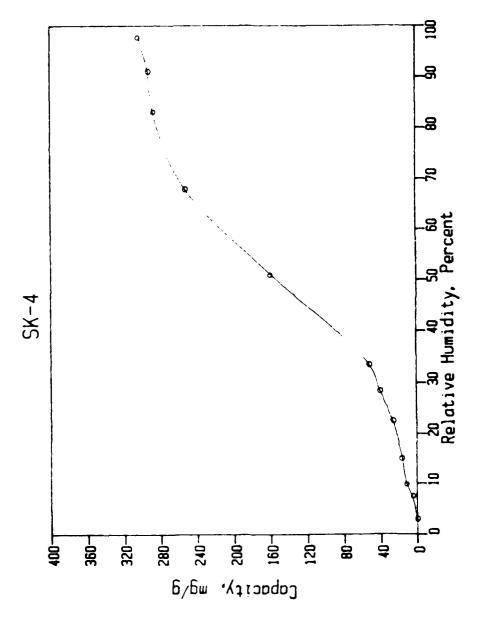
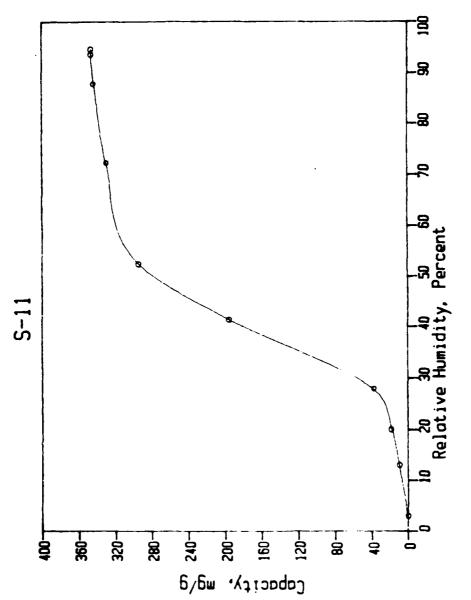
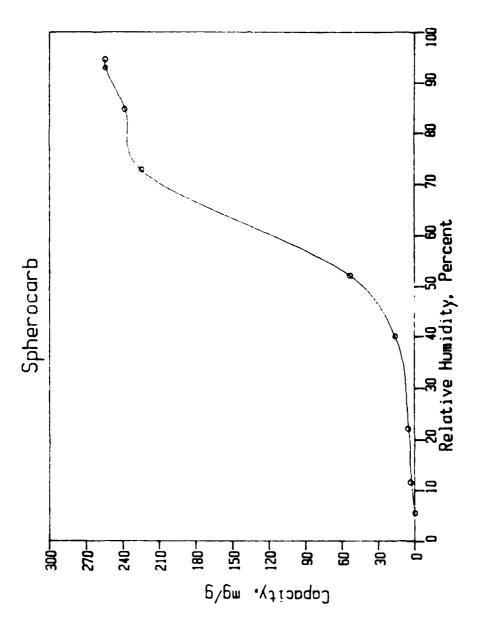


Figure B-1. Water Adsorption Isotherm SK-4.



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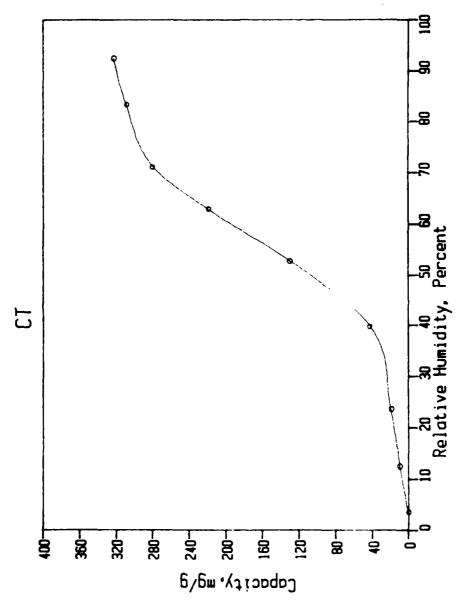
gure B-2. Water Adsorption Isotherm for Carbosieve S-11.



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Figure B-3. Water Adsorption Isotherm for Spherocarb.



igure B-4. Water Adsorption Isotherm for CT.

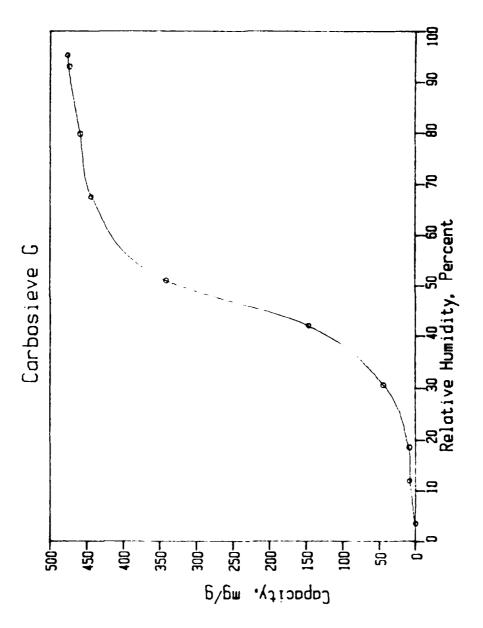


Figure B-5. Water Adsorption Isotherm for Carbosieve G.

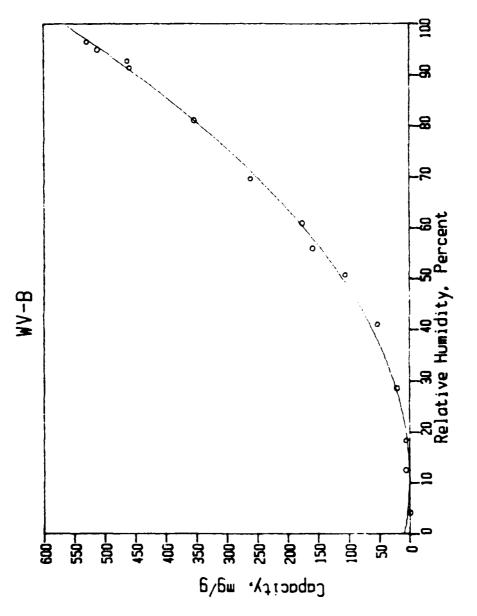


Figure B-6. Water Adsorption Isotherm for WV-B.

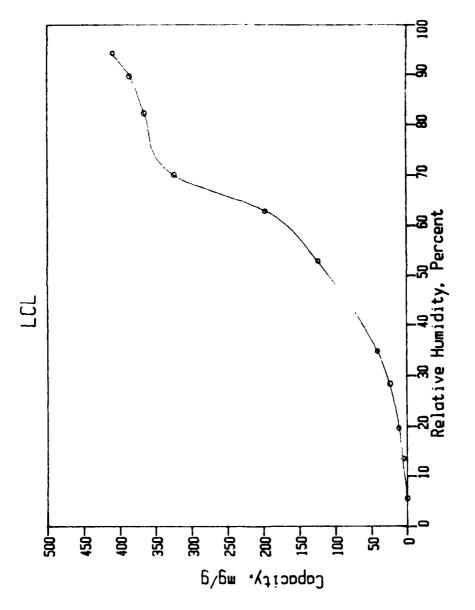


Figure B-7. Water Adsorption Isotherm for LCL.

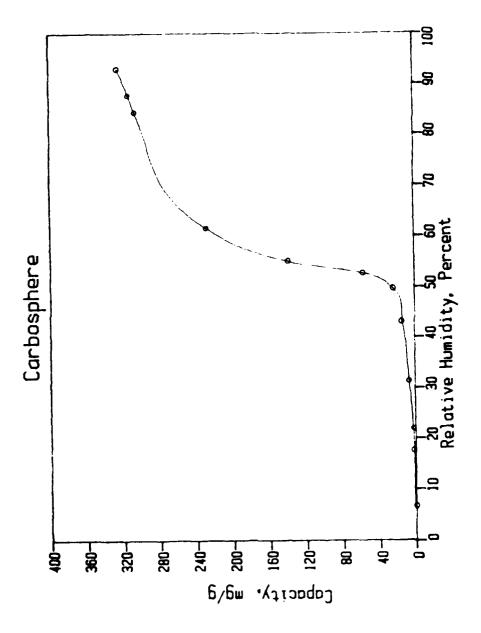


Figure B-8. Water Adsorption Isotherm for Carbosphere.

APPENDIX C

REFERENCE DATA

for

1,1-DICHLOROETHYLENE

S-11 S-11 S-11 S-11							
S-11 S-11 S-11	5 • x ~ m/6m	0, L/min	tios min meas cal	1 Dev. %	Capaci mg/ meas	T Dev.	% k, min ¹
S-11 S-11			1]	107		
			//2 /55 1466 1632	35 -2.16 32 11.33	107	15 -6.63 15 7.34	
Carbosieve S-II 30				'	122 157	'	
S-11					76		
S-11					82 91		7 15875
S-11 S-11					78		
S-11					44	49 11.97	
					9		
S-11 S-11	30 0.204 30 0.433	3 0.27	1291 1122 2729 2504	22 -13.11 04 -8.23	56 54	49 -12.03 49 -8.77	3 21064 7 16227
			Average	9.47	Average RMS	le <u>-2.56</u> 10.04	10 4
₩.	300 0.069 300 0.148	0.10		199 24.87 444 36.75	. 86	93 8.58 93 -0.66	
ਜ ਜ `			773 8			93 -15.11 93 4.92	2 10753
* *							
3 2							

TABLE C-1. SUMMARY OF DATA FOR 1,1-DICHLOROETHYLENE (CONTINUED)

	,	=		tios min	min in	8	Capacity mg/g	apacity, mg/g	» 30 0	k min1
Carbon	C, mg/m³	3	4. L/min	meas		חבי, א	meas	3	1	
CI	100	0.272	0.30	572	546	-4.58	99	64	-3.22	30750
CL	30	0.069	0.30	325	238	-26.12	20	6 5	-19.76	33424
55	ଚ୍ଚ ଚ	0.138	0.27	62 <i>/</i> 1456	609 1268	-2.90 -12.93	4 4	\$ \$	-4.4/	24388
				Average	age	3.40 18.64	Average RMS	age	-2.27 11.48	
3	000	600	0	178	197	10 76	67	73	9,10	10001
5K-4	900	0.194	0.10	411	446	8.44	78	23	-6.29	3424
SK-4	300	0.364	0.10	812	860	5.90	69	73	5.94	11226
2K-4	300	0.546	0.20	623	638	2.44	73	73	0.13	7247
SK-4	300	0.728	0.20	876	860	-1.84	75	73	-2.54	9044
SK-4	100	0.092	0.20	170	167	-1.72	45	48	6.34	14959
SK-4	100	0.194	0.25	180	318	76.83	41	48	16.72	3650
SK-4	100	0.364	0.30	528	528	-0.08	47	48	1.82	13677
SK-4	30	0.092	0.30	235	186	-20.87	34	5 8	-16.21	12385
SK-4	30	0.194	0.27	410	572	39.52	88	5 8	1.74	4490
SK-4	900	0.194	0.38	293	386	31.74	30	58	-5.04	5483
SK-4	98	0.364	0.27	1324	1166	-11.97	33	58	-13.67	9138
				Aver	Average	11.60 29.05	Average RMS	age	-0.16 9.37	

							Capacity	ity,		
Carbon	C, mg/m ³	3. D	Q, L/min	tion	cal	Dev, %	meas c	le l	Dev, %	k, min ¹
Carbosieve G	300	0.042	°	110	125	14.05	97	97	0.06	15415
	300	0.078	0	213	242	13.58	94	97	3.25	
	300	0.169	00	4/3	536	13.39	£ 6	, 6 7	12.80	
Carbosieve G	300	0.236	5 C	383 508	533	4.94	104	76	-6.67	5731
	001	0.042	0	95	110	16.05	55	62	12.77	
	100	0.078	0	167	174	3.90	61	6 2	1.67	
	100	0.169	0	333	329	-1.08	62	62	0.03	
	90	0.042	0	142	129	-9,33	ဆို ဒိ	36	-5.68	
	30	0.042	00	123	129	10.20	8 8 8	36	8.62 10.20	
Carbosieve G Carbosieve G	98	0.169	0.27	339 773	304 704	-10.30	39 6	36	-10.39	46053
				Ave	Average	3.64 10.28	Average RMS	age	0.54	
Spherocarb	300	0.091	0.10	208	232	11.38	85	86 86	1.25	6993
Spherocarb	300	0.353		1051		-6.44	06	98	-4.37	46125
Spherocarb	300	0.527		709		-33.07	82	8	1.25	-1649
Spherocarb	300	0.704		962		-33.08	84	86	2.46	-1129
Spherocarb	100	0.091		179		-35.77	2	2/	12.25	-25815
Spherocarb	100	0.175		281		21.73	51	2	12.25	8254
Spherocarb	901	0.353		040		-4.81	၉ :	ر در	77.7	23728

TABLE C-1. SUMMARY OF DATA FOR 1,1-DICHLOROETHYLENE (CONTINUED)

						·	Capacity,	tty.		
Carbon	C, mg/m ³	5	W, g Q, L/min	TIO MIN	Cal	Dev. %	meas	Cal	Dev, % k,	k, min ¹
Spherocarb Spherocarb Spherocarb	888	0.175 0.353 0.353	0.27 0.27 0.27	724 1588 1500	627 1384 1384	-13.47 -12.82 -7.70	38 33	35 35 35	-10.90 -8.56 -8.56	14226 27885 10829
				Ave	Average	-10.52 23.75	Average RMS	age	-0.95 10.21	

APPENDIX D

SINGLE-COMPONENT ADSORPTION DATA

TABLE D-1. SUMMARY OF SINGLE-COMPONENT DATA

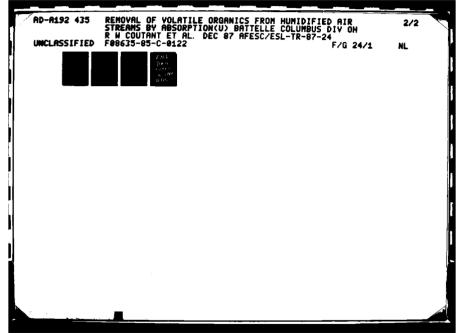
Carbon	C, mg/m³	5 *	Q, L/min	tin, min meas cal	min cal	Dev, %	Capacity, mq/q meas ca	ity,	Dev. X
			Benzene	ene					
Carboseive S-II Carbosieve S-II Carbosieve S-II Carbosieve S-II Carbosieve S-II Carcosieve S-II CI CI CI CI CI	300 100 300 300 100 38 300 100	0.651 0.222 0.222 0.212 0.204 0.433 0.136 0.136 0.138 0.272	0.272 0.1 0.3 0.3 0.28 0.1 0.3 0.3 0.3	1674 1542 1295 1187 1192 2369 5468 608 607 607 536 1187	1704 1577 1577 1175 1126 2528 6244 777 771 860 598 608 1274 3016	2.25 21.76 -1.02 -5.55 6.70 11.35 26.85 5.70 -1.46 13.44 7.32 6.89	213 222 195 183 187 174 174 166 142 145 116 116	220 220 220 220 184 184 1178 178 178 178 178 178 149 149 125 RNS	3.14 -1.04 12.67 0.36 -1.79 5.55 9.30 10.73 25.55 7.39 7.49 8.03 7.49
			Trichloroethylene	ethylene					
Carbosieve S-II Carbosieve S-II CT CT	30 30 30 30 30 30 30 30 30 30 30 30 30 3	0.108 0.204 0.069 0.138 0.138	0.225 0.32 0.225 0.3	484 4235 242 843 1789	464 4105 232 1096 2216	-4.08 -3.06 -4.06 30.07 23.86	354 212 286 286 185 135	337 216 274 215 175	-4.75 1.82 -4.32 16.25 29.88
	26	0.130	0.32	1/03	1777	,		73.80	73.80 135

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TABLE D-1. SUMMARY OF SINGLE-COMPONENT DATA (CONTINUED)

Carbon	C, mg/m ³	5°	Q, L/min	t ₁₀ , min meas ca	min cal	Dev, %	Capacity, mg/g meas ca	cal	Dev. %
SK-4 Carbosteve G SK-4	300 300	0.194 0.078 0.194	0.3 0.222 0.222	913 343 455	1216 355 604	33.14 3.49 32.74	127 320 199	181 334 237	42.91 4.29 19.32
				42	Average RMS	14.01 22.99	AVE RMS	Average RMS	13.18 22.15
			o-Xylene	lene					
*SK-4	30	0.194	0.342	3480	3167	-9.00	208	208 231	0.07
*Carbosieve S-II	300	0.204	0.333	973	604	-37.91 -31.68	511 423	332 269	-35.00
Carbosieve G	182	0.078	0.3	1230	434	-35.01	512 472	347 267	-32.24
Spherocarb	152	0.182	0.286	1720	925	-46.19	425	263	-38.00
Carbosieve 5-II	152 367	0.204	0.261	785	543 654	-16.72	403	336	-16.69
• • •	367	0.138	0.269	383	342	-10.75	333 243	272 218	-18.26
5K-4 CT	25 52	0.138	0.281	2490	2032	-18.40	330	241	-27.06
					Average RMS	-26.87 31.77	AV RM	Average RMS	-26.64 31.11

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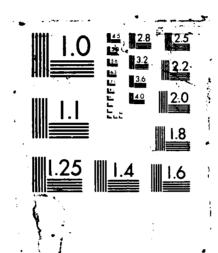


TABLE D-1. SUMMARY OF SINGLE-COMPONENT DATA (CONTINUED)

200	C. ma/m3	3	O. L/min	tln, min	min	Dev. %	Capacity mg/g	ity.	Dev, %
	: /6:: 1	,	orallo1						
			2	טוט					
*Suberncarh	300	0.175	0.214	267	549	-3,15	224	230	2.83
*Carbosieve G	300	0.078	0.214	333	328	-1.60	299	596	-1.05
*Carbosteve S-II	100	0.204	0,333	1469	1375	-6.39	258	252	-2.32
10 × 11 ×	100	0.138	0.333	715	741	3.59	215	204	-4.91
Carbosieve G	47	0.078	0.3	1297	1138	-12.25	592	235	-11.38
	53	0.175	0.3	2382	1719	-27.82	233	190	-18.66
Spherocarb	438	0.175	0.289	394	274	-30,39	307	239	-22.22
Spherocarb	407	0.182	0.29	448	306	-31.70	307	237	-22.75
Carbosieve G	438	0.078	0.3	210	160	-23.77	394	308	-21.87
	407	0.082	0.306	248	177	-28.64	408	306	-25.11
Carbosteve S-II	108	0.204	0.286	2053	1521	-25.92	332	254	-23.46
13	106	0.138	0.305	970	777	-19.90	280	506	-26.53
Spherocarb	49	0.182	0.288	2487	2028	-18.48	202	188	-7.11
				•	Average	-17.42	Ą	Average	-14.19
				_	RMS	21.82	₹	S	18.12
			Ethylbenzene	enzene					
*Carbosieve S-II	100	0.204	0.35	1853	1533	-17.28	344	297	-13.64
*SK-4	100	0.194	0.35	1043	970	-6.95	526	219	-3.16
*SK-4	300	0.194	0.24	672	551	-17.97	288	237	-17.67
*Spherocarb	300	0.175	0.24	882	551	-37.75	398	264	-33.74
Carbosieve G	63	0.078	0.305	1735	1075	-38.05	473	303	-35.95
Carbosieve S-II	71	0.204	0.305	3692	2456	-33.54	413	290	-29.86

SUMMARY OF SINGLE-COMPONENT DATA (CONCLUDED) TABLE D-1.

Carbon	C, mg/m ³	5 3	Q, L/min	tin, min meas cal	min	Dev, %	Capacity mg/g meas ca	ity.	0ev.,
Spherocarb SK-4 Carbosieve S-II SK-4	390 390 142 142		0.286 0.286 0.274 0.281	602 450 1630 955	367 351 1453 918	-39.05 -22.03 -10.88 -3.89	390 296 344 219	268 241 304 225	-31.27 -18.54 -11.50 2.69
				4 K	Average RMS	-22.74 27.51	A &	Average RMS	-19.26 24.25

*Possible error in concentration because of questionable sample preparation.

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